Full wwPDB EM Validation Report

Sep 8, 2026 – 11:55 pm BST

PDB ID	:	8S7V / pdb_00008s7v
EMDB ID	:	EMD-19787
Title	:	Methyl-coenzyme M reductase activation complex binding to the A2 component
Authors	:	Ramirez-Amador, F.; Paul, S.; Kumar, A.; Schuller, J.M.
Deposited on	:	2024-03-04
Resolution	:	2.56 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

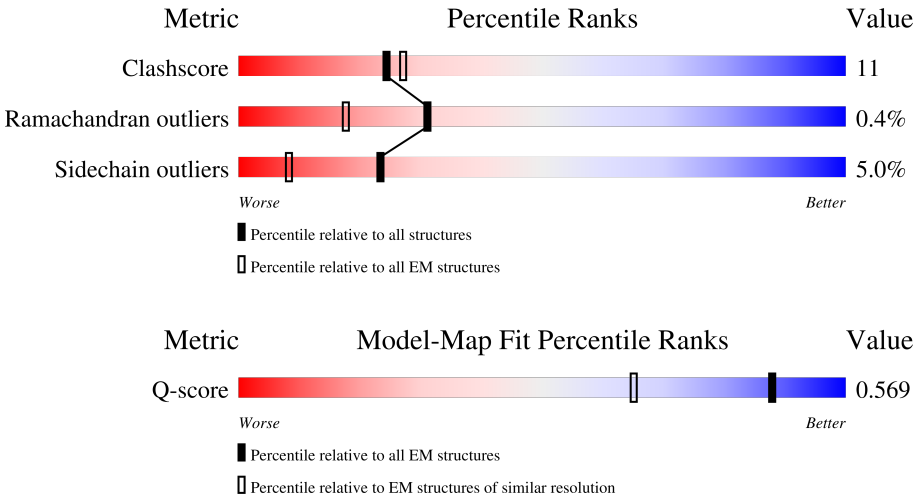
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7558 (2.06 - 3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	80% 19%
1	B	260	83% 17%
2	D	443	81% 18%
2	E	443	81% 18%

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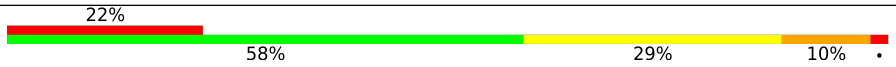
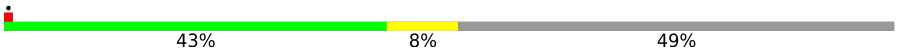
Mol	Chain	Length	Quality of chain
3	C	553	
3	F	553	
4	G	183	
5	H	304	
6	I	234	
7	K	531	
8	J	501	
9	L	93	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GL3	C	448	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		
1	B	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		
2	D	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	173	GLY	SER	conflict	UNP A0A2L1CBB3
D	173	GLY	SER	conflict	UNP A0A2L1CBB3

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	550	Total	C	N	O	S	0	0
			4284	2707	731	826	20		
3	F	520	Total	C	N	O	S	0	0
			4039	2556	684	779	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	SER	ALA	variant	UNP A0A2L1CBB0
F	51	SER	ALA	variant	UNP A0A2L1CBB0

- Molecule 4 is a protein called Methanogenesis marker protein 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	114	Total	C	N	O	S	0	0
			931	600	152	172	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	VAL	ILE	variant	UNP G0H411
G	129	ILE	VAL	variant	UNP G0H411
G	167	GLU	GLN	variant	UNP G0H411
G	168	GLU	ASP	variant	UNP G0H411
G	171	ASN	ASP	variant	UNP G0H411

- Molecule 5 is a protein called Methanogenesis marker protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	296	Total	C	N	O	S	0	0
			2393	1530	411	440	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	115	ASN	SER	variant	UNP G0H350
H	260	GLU	LYS	variant	UNP G0H350

- Molecule 6 is a protein called Methyl-coenzyme M reductase operon protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	194	Total	C	N	O	S	0	0
			1469	929	261	271	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-35	MET	-	initiating methionine	UNP G0H3B1
I	-34	SER	-	expression tag	UNP G0H3B1
I	-33	ALA	-	expression tag	UNP G0H3B1
I	-32	TRP	-	expression tag	UNP G0H3B1
I	-31	SER	-	expression tag	UNP G0H3B1
I	-30	HIS	-	expression tag	UNP G0H3B1
I	-29	PRO	-	expression tag	UNP G0H3B1
I	-28	GLN	-	expression tag	UNP G0H3B1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-27	PHE	-	expression tag	UNP G0H3B1
I	-26	GLU	-	expression tag	UNP G0H3B1
I	-25	LYS	-	expression tag	UNP G0H3B1
I	-24	GLY	-	expression tag	UNP G0H3B1
I	-23	GLY	-	expression tag	UNP G0H3B1
I	-22	GLY	-	expression tag	UNP G0H3B1
I	-21	SER	-	expression tag	UNP G0H3B1
I	-20	GLY	-	expression tag	UNP G0H3B1
I	-19	GLY	-	expression tag	UNP G0H3B1
I	-18	GLY	-	expression tag	UNP G0H3B1
I	-17	SER	-	expression tag	UNP G0H3B1
I	-16	GLY	-	expression tag	UNP G0H3B1
I	-15	GLY	-	expression tag	UNP G0H3B1
I	-14	SER	-	expression tag	UNP G0H3B1
I	-13	ALA	-	expression tag	UNP G0H3B1
I	-12	TRP	-	expression tag	UNP G0H3B1
I	-11	SER	-	expression tag	UNP G0H3B1
I	-10	HIS	-	expression tag	UNP G0H3B1
I	-9	PRO	-	expression tag	UNP G0H3B1
I	-8	GLN	-	expression tag	UNP G0H3B1
I	-7	PHE	-	expression tag	UNP G0H3B1
I	-6	GLU	-	expression tag	UNP G0H3B1
I	-5	LYS	-	expression tag	UNP G0H3B1
I	-4	SER	-	expression tag	UNP G0H3B1
I	-3	ALA	-	expression tag	UNP G0H3B1
I	-2	GLY	-	expression tag	UNP G0H3B1
I	-1	SER	-	expression tag	UNP G0H3B1
I	0	GLY	-	expression tag	UNP G0H3B1

- Molecule 7 is a protein called Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	521	Total	C	N	O	S	0	0
			4089	2598	693	774	24		

- Molecule 8 is a protein called UPF0288 protein MmarC6_0796.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	499	Total	C	N	O	S	0	0
			3962	2517	647	790	8		

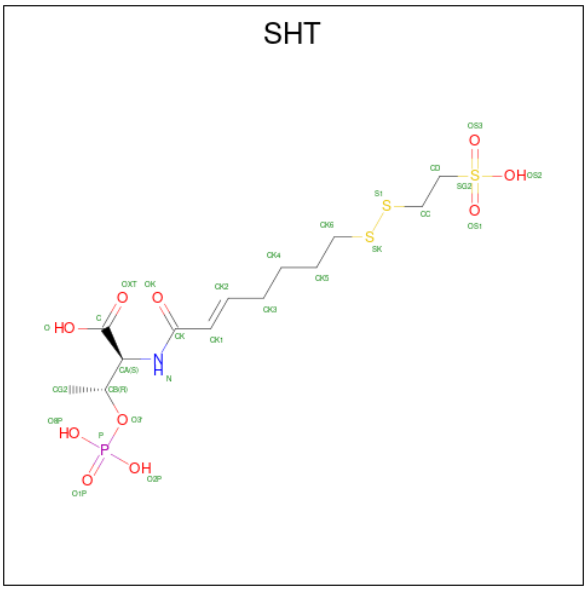
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	500	SER	LYS	variant	UNP A9A8E0

- Molecule 9 is a protein called DUF2098 domain-containing protein.

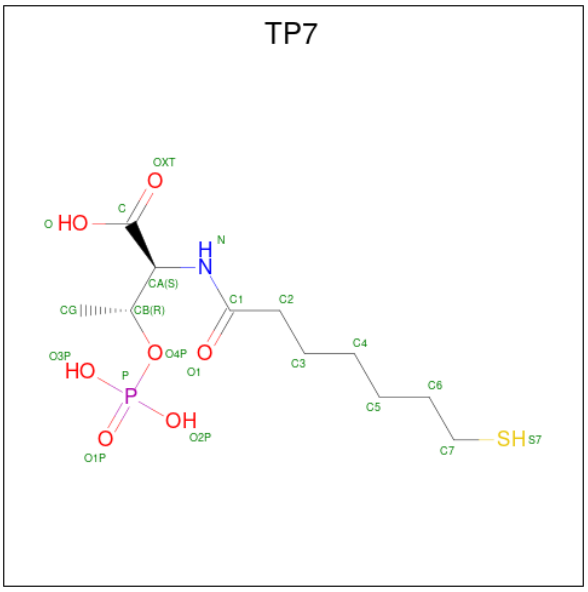
Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	47	Total	C	N	O	0	0
			390	251	61	78		

- Molecule 10 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (CCD ID: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$) (labeled as "Ligand of Interest" by depositor).



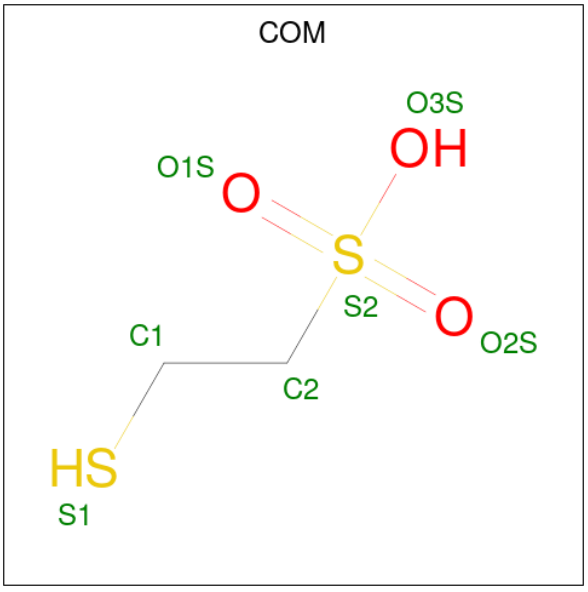
Mol	Chain	Residues	Atoms						AltConf
10	E	1	Total	C	N	O	P	S	0
			28	13	1	10	1	3	

- Molecule 11 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



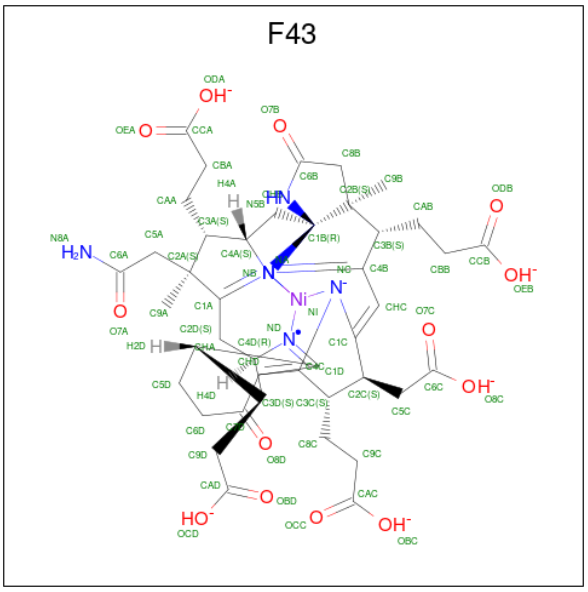
Mol	Chain	Residues	Atoms						AltConf
11	C	1	Total	C	N	O	P	S	0
			21	11	1	7	1	1	

- Molecule 12 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



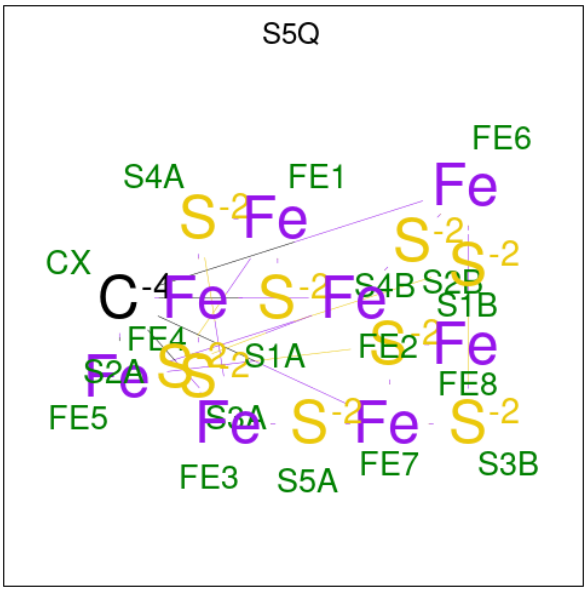
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	S	0
			7	2	3	2	

- Molecule 13 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



Mol	Chain	Residues	Atoms					AltConf
13	F	1	Total	C	N	Ni	O	0
			62	42	6	1	13	
13	F	1	Total	C	N	Ni	O	0
			62	42	6	1	13	

- Molecule 14 is FeFe cofactor (CCD ID: S5Q) (formula: CFe_8S_9) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	H	1	Total	C	Fe	S	0
			18	1	8	9	

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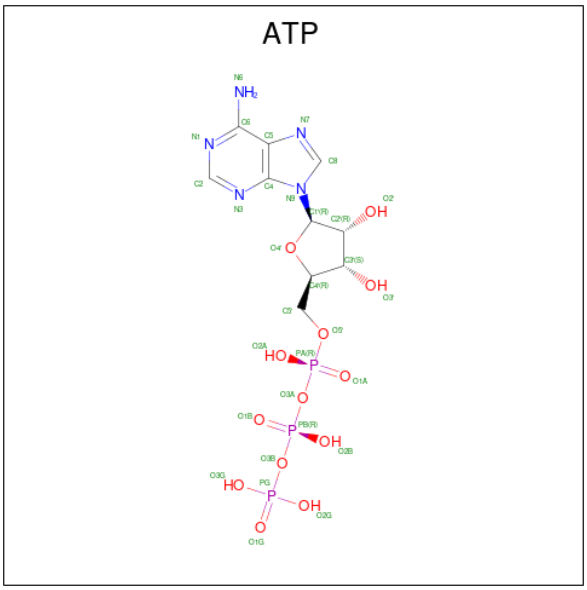
Mol	Chain	Residues	Atoms				AltConf
14	I	1	Total	C	Fe	S	0
			18	1	8	9	
14	I	1	Total	C	Fe	S	0
			18	1	8	9	

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	K	1	Total	Zn	0
			1	1	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

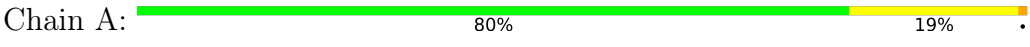
Mol	Chain	Residues	Atoms		AltConf
17	K	2	Total	Mg	0
			2	2	

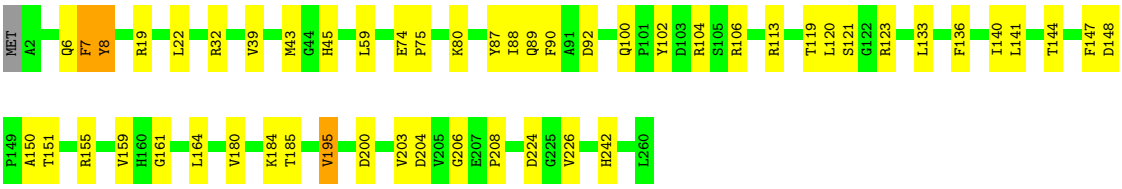
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Methyl-coenzyme M reductase subunit gamma

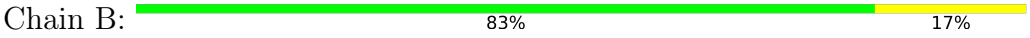
Chain A:

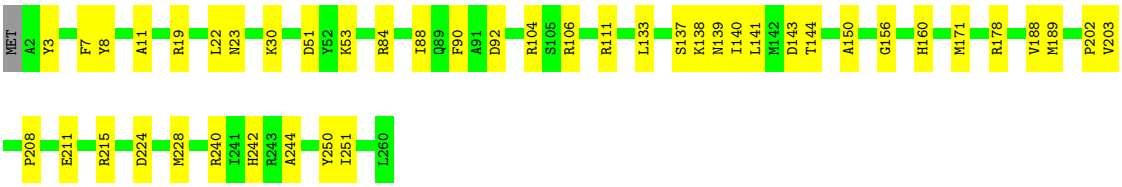




• Molecule 1: Methyl-coenzyme M reductase subunit gamma

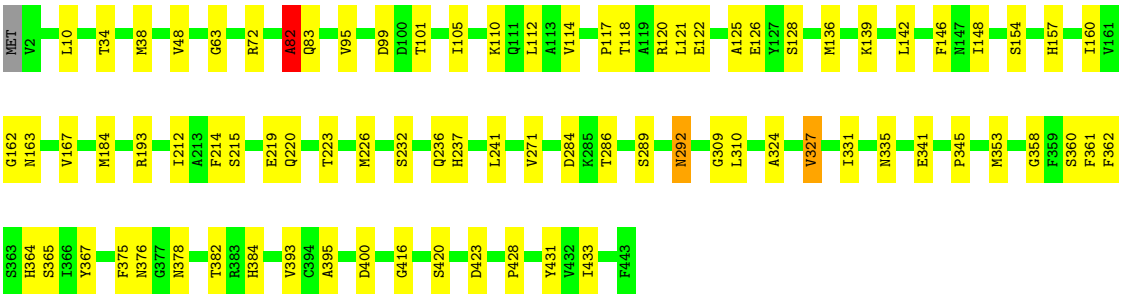
Chain B:





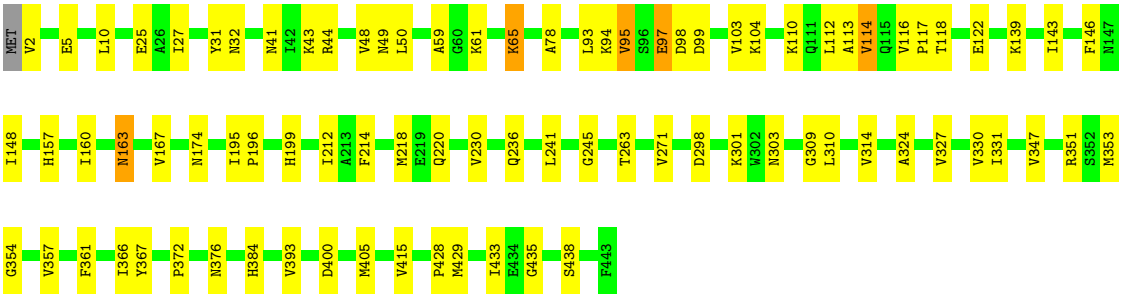
• Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain E:



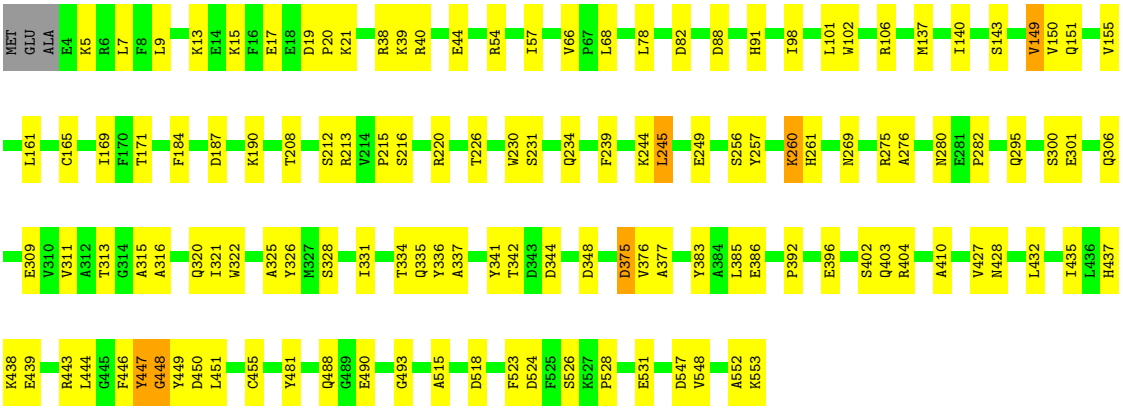
• Molecule 2: Methyl-coenzyme M reductase subunit beta

Chain D:



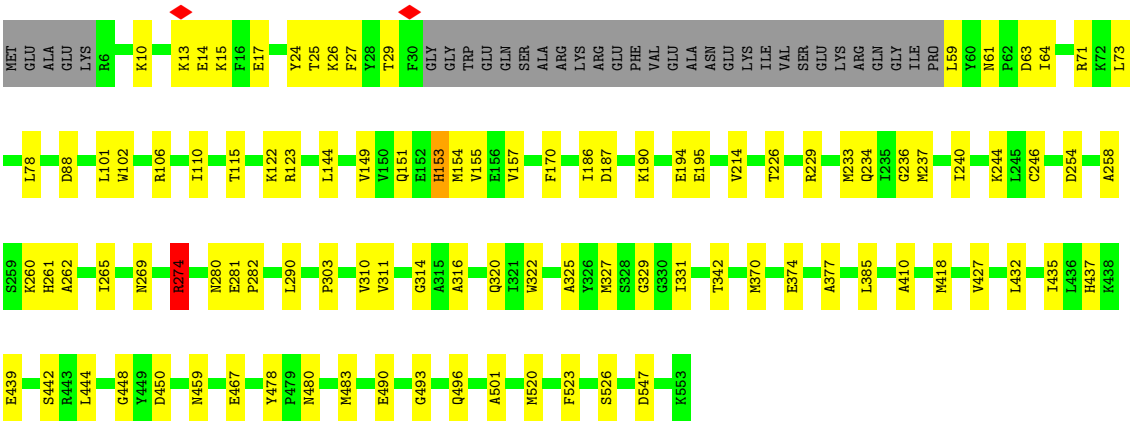
• Molecule 3: Methyl-coenzyme M reductase subunit alpha

Chain C:



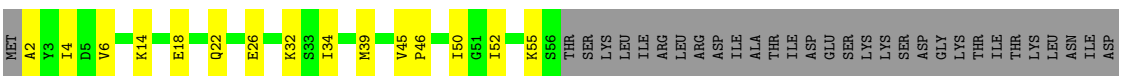
• Molecule 3: Methyl-coenzyme M reductase subunit alpha

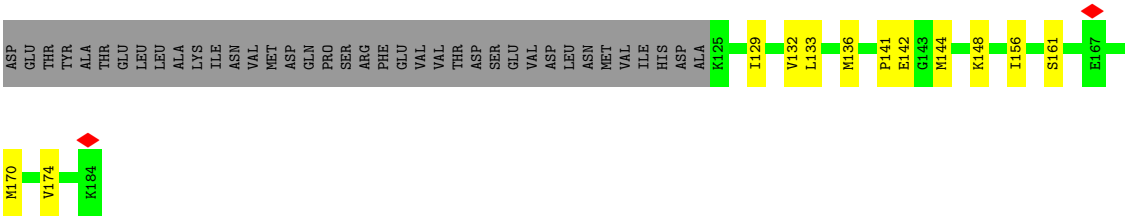
Chain F:



• Molecule 4: Methanogenesis marker protein 17

Chain G:



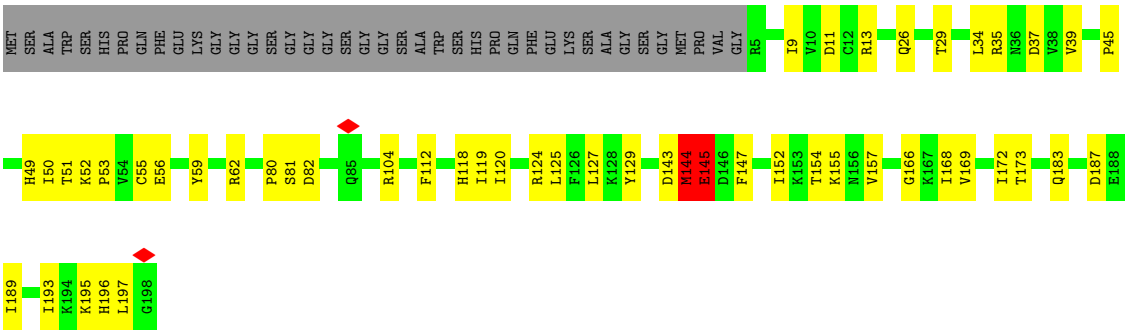


• Molecule 5: Methanogenesis marker protein 7

Chain H:

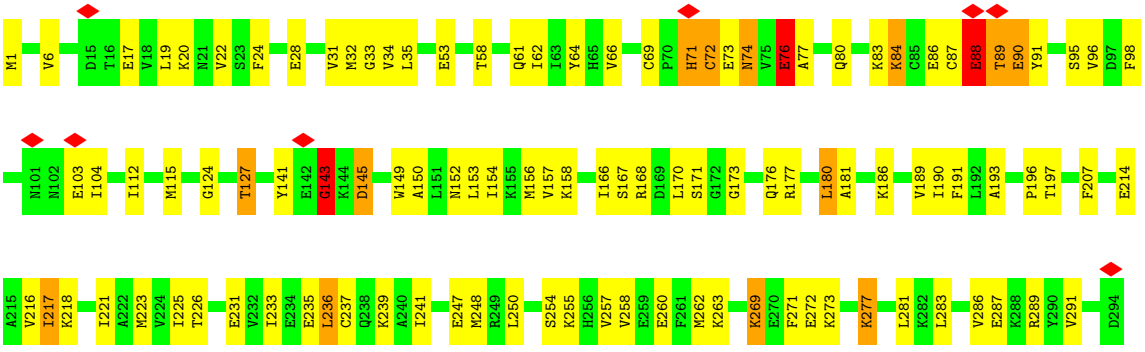
• Molecule 6: Methyl-coenzyme M reductase operon protein C

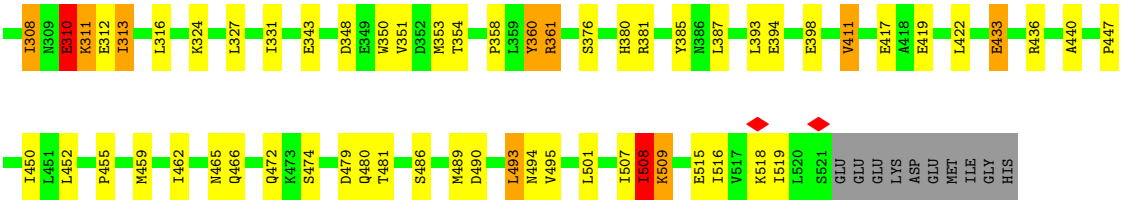
Chain I:



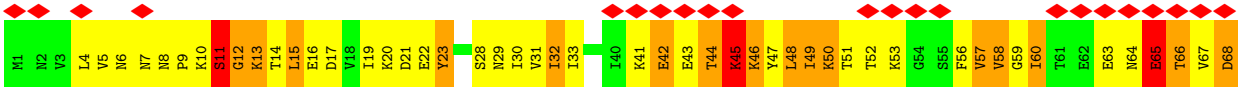
• Molecule 7: Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA

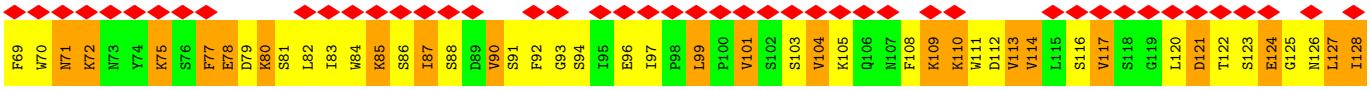
Chain K:

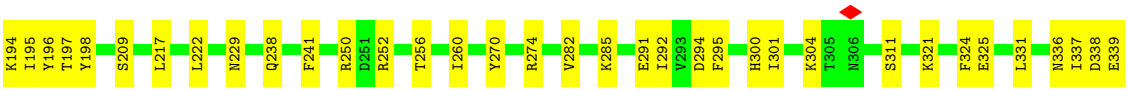


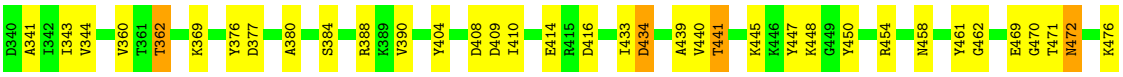


• Molecule 8: UPF0288 protein MmarC6_0796

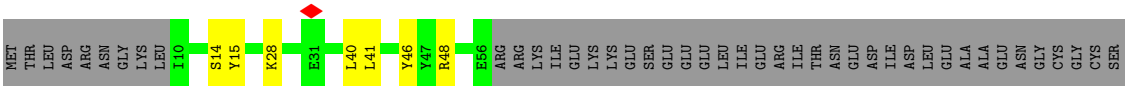








• Molecule 9: DUF2098 domain-containing protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	484016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.051	Depositor
Map size (Å)	350.40002, 350.40002, 350.40002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7300001, 0.7300001, 0.7300001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MGN, COM, MHS, MG, S5Q, AGM, ATP, TP7, GL3, F43, ZN, SHT, SMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.20	0/2116	0.48	3/2861 (0.1%)
1	B	0.20	0/2116	0.34	0/2861
2	D	0.16	0/3319	0.42	6/4499 (0.1%)
2	E	0.19	0/3319	0.50	6/4499 (0.1%)
3	C	0.22	0/4328	0.38	0/5856
3	F	0.16	0/4078	0.35	1/5522 (0.0%)
4	G	0.12	0/943	0.30	0/1262
5	H	0.17	0/2435	0.37	0/3280
6	I	0.24	0/1490	0.60	3/2006 (0.1%)
7	K	0.33	0/4159	0.83	25/5613 (0.4%)
8	J	0.53	0/4026	1.02	10/5441 (0.2%)
9	L	0.11	0/398	0.35	0/542
All	All	0.27	0/32727	0.59	54/44242 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
7	K	0	2
8	J	0	6
All	All	0	10

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	32	ILE	O-C-N	32.65	156.66	123.03
8	J	32	ILE	CA-C-N	-21.57	87.91	122.64
8	J	32	ILE	C-N-CA	-21.57	87.91	122.64
8	J	179	TYR	CA-C-N	-20.16	91.16	122.81
8	J	179	TYR	C-N-CA	-20.16	91.16	122.81
7	K	88	GLU	CB-CA-C	-20.10	73.20	109.38
8	J	179	TYR	O-C-N	13.66	140.20	123.26
7	K	360	TYR	N-CA-C	13.45	139.46	110.80
2	E	82	ALA	CB-CA-C	-12.37	85.80	110.42
2	D	163	ASN	N-CA-C	11.63	127.42	113.23
6	I	145	GLU	N-CA-CB	-11.13	91.91	110.39
6	I	145	GLU	N-CA-C	11.10	126.08	112.54
2	E	83	GLN	N-CA-C	-10.97	87.44	110.80
7	K	90	GLU	N-CA-CB	-10.82	92.20	110.49
7	K	73	GLU	N-CA-C	10.76	128.52	113.56
2	E	63	GLY	N-CA-C	10.36	129.92	115.00
1	A	7	PHE	N-CA-C	-10.33	92.72	108.00
7	K	91	TYR	N-CA-CB	-10.25	96.73	110.57
1	A	8	TYR	N-CA-C	10.25	125.76	110.39
1	A	8	TYR	N-CA-CB	-10.04	95.93	109.78
6	I	144	MET	CB-CA-C	9.97	127.63	110.68
7	K	91	TYR	N-CA-C	9.27	124.70	108.56
7	K	509	LYS	N-CA-CB	-9.22	96.65	110.85
8	J	43	GLU	N-CA-C	-8.62	103.35	114.04
7	K	508	ILE	N-CA-C	-8.59	91.47	109.34
3	F	153	HIS	N-CA-C	-8.47	92.76	110.80
7	K	433	GLU	N-CA-C	-8.44	103.50	113.88
7	K	361	ARG	N-CA-C	-8.41	92.89	110.80
2	E	83	GLN	N-CA-CB	8.22	124.39	110.49
7	K	74	ASN	N-CA-CB	-8.18	97.10	110.43
7	K	143	GLY	N-CA-C	8.10	132.39	113.18
7	K	74	ASN	N-CA-C	7.88	122.08	109.24
7	K	89	THR	CB-CA-C	-7.63	95.24	110.42
7	K	77	ALA	N-CA-C	-7.34	100.78	110.40
7	K	88	GLU	CA-C-N	7.28	135.44	121.54
7	K	88	GLU	C-N-CA	7.28	135.44	121.54
8	J	45	LYS	N-CA-C	-7.01	102.85	111.33
2	E	82	ALA	N-CA-C	6.90	125.50	110.80
7	K	76	GLU	CB-CA-C	6.61	123.57	110.42
7	K	361	ARG	N-CA-CB	6.45	121.39	110.49
7	K	127	THR	N-CA-C	6.07	116.99	108.00
7	K	143	GLY	CA-C-N	6.05	131.80	122.42
7	K	143	GLY	C-N-CA	6.05	131.80	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	360	TYR	CB-CA-C	-5.95	98.59	110.42
2	D	98	ASP	N-CA-C	5.83	119.45	112.93
2	D	98	ASP	N-CA-CB	-5.81	102.54	110.56
2	E	232	SER	N-CA-C	5.80	119.45	112.38
7	K	90	GLU	CB-CA-C	-5.73	99.01	110.42
8	J	145	ILE	N-CA-C	-5.70	107.29	111.90
7	K	509	LYS	N-CA-C	5.65	118.90	110.14
8	J	65	GLU	N-CA-C	-5.26	106.64	114.64
2	D	97	GLU	CB-CA-C	5.07	120.51	110.42
2	D	95	VAL	CA-C-N	-5.02	115.57	121.90
2	D	95	VAL	C-N-CA	-5.02	115.57	121.90

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	447	TYR	Mainchain
3	F	274	ARG	Sidechain
8	J	132	ARG	Sidechain
8	J	153	ARG	Sidechain
8	J	163	ARG	Sidechain
8	J	171	ARG	Sidechain
8	J	179	TYR	Mainchain
8	J	42	GLU	Mainchain
7	K	143	GLY	Peptide
7	K	88	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2071	0	2012	42	0
1	B	2071	0	2012	29	0
2	D	3263	0	3260	61	0
2	E	3263	0	3260	53	0
3	C	4284	0	4147	108	0
3	F	4039	0	3904	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	931	0	970	19	0
5	H	2393	0	2475	57	0
6	I	1469	0	1534	34	0
7	K	4089	0	4162	104	0
8	J	3962	0	3996	191	0
9	L	390	0	378	5	0
10	E	28	0	21	2	0
11	C	21	0	19	1	0
12	C	7	0	5	1	0
13	F	124	0	86	15	0
14	H	18	0	0	1	0
14	I	36	0	0	0	0
15	K	1	0	0	0	0
16	K	62	0	24	2	0
17	K	2	0	0	0	0
All	All	32524	0	32265	690	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (690) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:179:TYR:CE1	8:J:295:PHE:HB3	1.36	1.56
3:C:447:TYR:C	3:C:448:GL3:CA	1.86	1.49
3:C:447:TYR:CA	3:C:448:GL3:N	1.84	1.39
8:J:179:TYR:CD1	8:J:295:PHE:HB3	1.61	1.34
8:J:179:TYR:CE1	8:J:295:PHE:CB	2.16	1.28
8:J:42:GLU:HA	8:J:172:GLU:HB3	1.24	1.16
3:C:447:TYR:O	3:C:448:GL3:N	1.87	1.07
8:J:96:GLU:HA	8:J:123:SER:HA	1.37	1.06
8:J:117:VAL:HA	8:J:125:GLY:HA2	1.41	1.02
8:J:170:MET:HE1	8:J:172:GLU:OE1	1.59	1.01
7:K:127:THR:O	7:K:167:SER:HB3	1.60	1.01
8:J:179:TYR:CZ	8:J:295:PHE:HB3	1.96	1.00
5:H:209:GLU:CG	8:J:149:ILE:CD1	2.42	0.97
8:J:179:TYR:CD1	8:J:295:PHE:CB	2.40	0.96
5:H:209:GLU:HG2	8:J:149:ILE:CD1	1.93	0.96
8:J:170:MET:CE	8:J:172:GLU:OE1	2.15	0.95
3:C:447:TYR:C	3:C:448:GL3:N	0.84	0.94
8:J:44:THR:HG21	8:J:169:GLN:HB2	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:99:LEU:HG	8:J:141:GLU:OE2	1.66	0.93
8:J:33:ILE:HG12	8:J:196:TYR:HE1	1.30	0.93
2:D:357:VAL:O	3:C:448:GL3:HA1	1.70	0.91
5:H:209:GLU:CG	8:J:149:ILE:HD13	2.00	0.91
2:E:82:ALA:O	2:E:105:ILE:CD1	2.18	0.90
2:D:357:VAL:O	3:C:448:GL3:CA	2.21	0.89
2:E:367:TYR:OH	13:F:601:F43:H5A2	1.72	0.89
7:K:351:VAL:CG2	7:K:360:TYR:O	2.23	0.86
3:C:447:TYR:C	3:C:448:GL3:HA2	2.01	0.85
5:H:209:GLU:HG2	8:J:149:ILE:HG12	1.57	0.85
5:H:209:GLU:HG3	8:J:149:ILE:HD13	1.57	0.85
5:H:209:GLU:HG3	8:J:149:ILE:CD1	2.06	0.85
5:H:209:GLU:HG2	8:J:149:ILE:CG1	2.07	0.84
8:J:42:GLU:CA	8:J:172:GLU:HB3	2.08	0.84
3:C:447:TYR:O	3:C:448:GL3:CA	2.18	0.83
8:J:99:LEU:HB3	8:J:140:LEU:HD11	1.62	0.82
8:J:46:LYS:HA	8:J:59:GLY:HA2	1.61	0.81
8:J:155:LEU:HA	8:J:158:LEU:HD12	1.62	0.81
7:K:283:LEU:HD23	7:K:286:VAL:HG21	1.63	0.80
8:J:168:GLU:HG2	8:J:171:ARG:HH12	1.45	0.80
8:J:170:MET:HE3	8:J:172:GLU:HB2	1.65	0.78
3:C:447:TYR:CB	3:C:448:GL3:N	2.47	0.77
8:J:33:ILE:HG12	8:J:196:TYR:CE1	2.18	0.76
2:D:357:VAL:HG12	3:C:448:GL3:HA2	1.66	0.76
8:J:47:TYR:HB2	8:J:58:VAL:HG22	1.68	0.76
7:K:191:PHE:HB3	7:K:223:MET:HG2	1.69	0.75
8:J:101:VAL:HA	8:J:140:LEU:HA	1.68	0.75
8:J:84:TRP:HD1	8:J:86:SER:H	1.35	0.75
8:J:321:LYS:HD3	8:J:331:LEU:HD13	1.68	0.75
2:E:82:ALA:O	2:E:105:ILE:HD11	1.87	0.74
3:C:257:TYR:HA	3:C:261:MHS:HD2	1.69	0.74
2:D:48:VAL:HB	2:D:112:LEU:HB2	1.69	0.74
8:J:179:TYR:CE1	8:J:295:PHE:HB2	2.23	0.74
1:A:102:TYR:CE1	1:A:119:THR:HG21	2.22	0.74
8:J:179:TYR:OH	8:J:181:ILE:HB	1.88	0.73
2:E:223:THR:HA	2:E:226:MET:HE2	1.69	0.73
8:J:81:SER:HA	8:J:163:ARG:HA	1.70	0.73
3:C:447:TYR:O	3:C:448:GL3:HA2	1.87	0.73
7:K:452:LEU:HB3	7:K:455:PRO:HG3	1.69	0.72
2:E:99:ASP:OD1	2:E:101:THR:OG1	2.06	0.71
5:H:225:GLU:HG2	5:H:267:ILE:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:216:VAL:HG11	7:K:223:MET:HG3	1.72	0.71
8:J:65:GLU:HG3	8:J:141:GLU:OE2	1.90	0.71
7:K:1:MET:SD	7:K:1:MET:N	2.63	0.71
7:K:88:GLU:O	7:K:89:THR:HG23	1.90	0.70
5:H:209:GLU:CG	8:J:149:ILE:HD11	2.21	0.70
8:J:179:TYR:CD1	8:J:295:PHE:CG	2.78	0.70
7:K:351:VAL:HG21	7:K:360:TYR:O	1.91	0.70
2:D:220:GLN:HG3	2:D:241:LEU:HB2	1.74	0.70
3:C:155:VAL:HG13	3:F:88:ASP:HA	1.74	0.70
8:J:82:LEU:HB3	8:J:160:ALA:HA	1.74	0.70
1:A:140:ILE:O	1:A:144:THR:OG1	2.10	0.70
8:J:33:ILE:CG1	8:J:196:TYR:HE1	2.03	0.69
1:B:7:PHE:HB2	1:B:19:ARG:HG2	1.74	0.69
3:C:17:GLU:OE1	3:C:17:GLU:N	2.15	0.69
3:F:122:LYS:HE3	3:F:123:ARG:HG3	1.74	0.69
8:J:42:GLU:HA	8:J:172:GLU:CB	2.15	0.69
8:J:170:MET:CE	8:J:172:GLU:HB2	2.23	0.69
8:J:153:ARG:HE	8:J:154:VAL:HG23	1.57	0.69
2:D:357:VAL:O	3:C:448:GL3:HA2	1.93	0.68
3:C:403:MGN:NE2	13:F:602:F43:H6D2	2.08	0.68
3:F:331:ILE:HB	13:F:601:F43:C9A	2.24	0.68
8:J:440:VAL:O	8:J:472:ASN:ND2	2.27	0.68
8:J:22:GLU:HB3	8:J:197:THR:HG21	1.74	0.68
2:E:212:ILE:HD11	2:E:395:ALA:HB2	1.76	0.67
2:D:303:ASN:ND2	2:D:347:VAL:O	2.27	0.67
7:K:489:MET:HE3	7:K:489:MET:HA	1.76	0.66
3:C:91:HIS:NE2	3:C:331:ILE:O	2.27	0.66
7:K:216:VAL:HG13	7:K:221:ILE:HB	1.78	0.66
5:H:71:ILE:HD13	5:H:203:ILE:HG12	1.77	0.66
3:F:459:ASN:ND2	3:F:480:ASN:OD1	2.28	0.66
8:J:56:PHE:HA	8:J:151:GLY:HA3	1.77	0.66
8:J:179:TYR:CZ	8:J:181:ILE:HB	2.31	0.66
5:H:88:ILE:HD11	5:H:179:ARG:HB2	1.78	0.65
2:D:353:MET:O	2:D:357:VAL:HG23	1.96	0.65
2:E:376:ASN:O	2:E:382:THR:OG1	2.13	0.65
5:H:256:ASP:OD1	5:H:280:ARG:NH2	2.29	0.65
8:J:49:ILE:HA	8:J:168:GLU:H	1.62	0.65
8:J:5:VAL:H	8:J:9:PRO:HA	1.62	0.64
7:K:157:VAL:HG11	7:K:181:ALA:HB2	1.80	0.64
2:E:367:TYR:OH	13:F:601:F43:C5A	2.47	0.63
2:E:48:VAL:HB	2:E:112:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:46:PRO:HG3	5:H:114:LYS:HD3	1.80	0.63
7:K:507:ILE:O	7:K:508:ILE:C	2.42	0.63
8:J:222:LEU:HD23	8:J:301:ILE:HD11	1.80	0.63
1:B:150:ALA:HB2	1:B:208:PRO:HB3	1.81	0.63
8:J:23:TYR:CE2	8:J:304:LYS:HB2	2.34	0.63
8:J:110:LYS:HG2	8:J:132:ARG:HA	1.80	0.63
7:K:71:HIS:CE1	7:K:88:GLU:O	2.52	0.63
1:A:92:ASP:OD1	1:A:104:ARG:NH1	2.32	0.62
6:I:51:THR:HA	6:I:55:CYS:HB2	1.81	0.62
8:J:97:ILE:HG13	8:J:125:GLY:HA3	1.80	0.62
7:K:34:VAL:HB	7:K:226:THR:HG22	1.81	0.62
2:E:82:ALA:O	2:E:105:ILE:HD12	2.00	0.62
7:K:260:GLU:HA	7:K:263:LYS:HE3	1.82	0.62
8:J:112:ASP:HA	8:J:147:ILE:HA	1.81	0.62
1:A:7:PHE:HB2	1:A:19:ARG:HG2	1.81	0.62
7:K:71:HIS:ND1	7:K:88:GLU:O	2.32	0.62
6:I:195:LYS:HD2	6:I:196:HIS:CD2	2.34	0.61
3:F:237:MET:HE2	13:F:602:F43:HBA1	1.82	0.61
6:I:52:LYS:HA	6:I:52:LYS:HE2	1.83	0.61
8:J:29:ASN:OD1	8:J:300:HIS:O	2.19	0.61
8:J:101:VAL:HG11	8:J:120:LEU:HA	1.83	0.61
8:J:79:ASP:HA	8:J:165:ILE:HA	1.82	0.61
8:J:96:GLU:CA	8:J:123:SER:HA	2.23	0.61
8:J:78:GLU:HA	8:J:167:ILE:HG13	1.82	0.61
2:D:5:GLU:OE2	2:D:5:GLU:N	2.22	0.60
4:G:129:ILE:O	4:G:133:LEU:HG	2.01	0.60
6:I:155:LYS:O	9:L:48:ARG:NH2	2.34	0.60
7:K:115:MET:HE1	7:K:180:LEU:HD23	1.81	0.60
4:G:34:ILE:HD13	4:G:52:ILE:HD12	1.84	0.60
7:K:287:GLU:OE2	7:K:289:ARG:NH1	2.34	0.60
8:J:22:GLU:C	8:J:23:TYR:N	2.59	0.60
3:C:187:ASP:HB3	3:C:190:LYS:HG2	1.84	0.60
9:L:40:LEU:HD23	9:L:46:TYR:CD1	2.36	0.60
7:K:351:VAL:HG22	7:K:360:TYR:O	2.02	0.60
2:E:220:GLN:HG3	2:E:241:LEU:HB2	1.83	0.60
4:G:142:GLU:OE1	5:H:81:SER:OG	2.16	0.60
1:A:32:ARG:NH2	1:A:144:THR:O	2.34	0.60
3:F:71:ARG:O	3:F:71:ARG:NH1	2.33	0.60
7:K:158:LYS:HG3	7:K:207:PHE:CD2	2.36	0.60
2:E:292:ASN:OD1	2:E:292:ASN:N	2.35	0.59
3:C:377:ALA:HB3	3:C:432:LEU:HD23	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:51:THR:HG21	8:J:158:LEU:HD11	1.84	0.59
8:J:41:LYS:O	8:J:172:GLU:O	2.19	0.59
3:F:377:ALA:HB3	3:F:432:LEU:HD23	1.83	0.59
6:I:56:GLU:HA	6:I:59:TYR:CE2	2.37	0.59
5:H:183:LEU:HD22	5:H:188:GLU:HB3	1.85	0.59
7:K:507:ILE:HG23	7:K:508:ILE:O	2.03	0.58
1:A:87:TYR:CZ	3:F:246:CYS:HB2	2.38	0.58
1:B:92:ASP:OD1	1:B:104:ARG:NH1	2.36	0.58
7:K:31:VAL:HB	7:K:237:CYS:HA	1.84	0.58
7:K:447:PRO:HG2	7:K:450:ILE:HG12	1.85	0.58
8:J:4:LEU:HD12	8:J:9:PRO:HB3	1.83	0.58
4:G:170:MET:O	4:G:174:VAL:HG23	2.03	0.58
3:F:106:ARG:O	3:F:280:ASN:ND2	2.35	0.58
7:K:509:LYS:HD3	7:K:519:ILE:HG13	1.83	0.58
1:B:23:ASN:O	1:B:111:ARG:NH1	2.36	0.58
4:G:39:MET:HG3	4:G:50:ILE:HG12	1.84	0.58
5:H:72:GLU:OE2	5:H:245:GLN:NE2	2.36	0.58
1:A:120:LEU:HD21	3:C:447:TYR:CD2	2.38	0.58
8:J:445:LYS:NZ	8:J:469:GLU:OE2	2.37	0.58
1:B:156:GLY:O	1:B:178:ARG:NH2	2.37	0.58
4:G:46:PRO:O	4:G:161:SER:OG	2.20	0.58
7:K:153:LEU:HA	7:K:156:MET:HG3	1.86	0.58
7:K:490:ASP:OD1	7:K:490:ASP:N	2.37	0.58
5:H:25:GLY:HA3	8:J:274:ARG:HD2	1.86	0.57
4:G:141:PRO:HG2	4:G:144:MET:HG2	1.85	0.57
2:D:104:LYS:HG3	2:D:113:ALA:HB3	1.86	0.57
3:C:171:THR:HB	3:C:208:THR:HG23	1.86	0.57
8:J:33:ILE:HD11	8:J:196:TYR:OH	2.04	0.57
8:J:324:PHE:HD2	8:J:331:LEU:HD21	1.70	0.57
2:E:335:ASN:HB3	2:E:353:MET:HE2	1.86	0.57
7:K:436:ARG:HG3	7:K:459:MET:HE1	1.86	0.57
3:C:106:ARG:O	3:C:280:ASN:ND2	2.30	0.57
1:A:123:ARG:HG2	1:A:159:VAL:HG21	1.87	0.57
4:G:132:VAL:HG11	4:G:156:ILE:HD12	1.86	0.57
6:I:26:GLN:O	6:I:29:THR:OG1	2.21	0.57
1:B:30:LYS:HA	1:B:144:THR:HA	1.87	0.56
8:J:179:TYR:CG	8:J:295:PHE:HB3	2.33	0.56
1:B:244:ALA:HB1	2:E:345:PRO:HG3	1.86	0.56
5:H:73:ILE:HG23	5:H:132:ILE:HG23	1.86	0.56
5:H:257:ARG:HB2	5:H:257:ARG:NH1	2.21	0.56
1:A:32:ARG:NH2	1:A:147:PHE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ALA:HB2	2:E:289:SER:HB3	1.87	0.56
5:H:179:ARG:NH1	5:H:188:GLU:OE2	2.39	0.56
2:E:34:THR:O	2:E:38:MET:HG3	2.06	0.56
5:H:295:SER:OG	5:H:296:GLU:OE1	2.24	0.56
1:B:139:ASN:OD1	7:K:381:ARG:NH2	2.35	0.56
8:J:148:LEU:HG	8:J:155:LEU:HD22	1.87	0.56
8:J:445:LYS:HE2	8:J:470:GLY:HA3	1.87	0.56
4:G:55:LYS:NZ	3:F:547:ASP:O	2.28	0.55
3:F:303:PRO:HB2	3:F:418:MET:HE1	1.89	0.55
7:K:311:LYS:HG3	7:K:479:ASP:HA	1.89	0.55
2:D:196:PRO:HA	2:D:376:ASN:HB3	1.88	0.55
3:F:15:LYS:O	8:J:404:TYR:OH	2.23	0.55
7:K:255:LYS:HA	7:K:255:LYS:HE3	1.88	0.55
8:J:49:ILE:HG13	8:J:167:ILE:HA	1.88	0.55
8:J:390:VAL:HG23	8:J:416:ASP:HB2	1.88	0.55
1:A:120:LEU:HB3	13:F:602:F43:O8C	2.06	0.55
3:C:300:SER:O	3:C:306:GLN:NE2	2.39	0.55
1:A:242:HIS:HB2	3:C:435:ILE:HD11	1.89	0.55
8:J:250:ARG:NH1	8:J:270:TYR:OH	2.39	0.55
8:J:70:TRP:O	8:J:71:ASN:C	2.50	0.55
3:C:322:TRP:O	3:C:326:TYR:HB2	2.06	0.54
3:F:520:MET:HE3	3:F:520:MET:HA	1.89	0.54
6:I:183:GLN:NE2	6:I:187:ASP:OD1	2.33	0.54
8:J:252:ARG:O	8:J:285:LYS:NZ	2.40	0.54
1:B:140:ILE:O	1:B:144:THR:OG1	2.22	0.54
3:C:315:ALA:HB1	3:C:337:ALA:HB1	1.89	0.54
8:J:32:ILE:HD11	8:J:195:ILE:HB	1.89	0.54
2:D:357:VAL:HG12	3:C:448:GL3:CA	2.37	0.54
1:B:3:TYR:OH	2:E:341:GLU:OE1	2.24	0.54
8:J:441:THR:OG1	8:J:447:TYR:O	2.24	0.54
3:C:213:ARG:NH2	3:C:515:ALA:O	2.37	0.53
1:A:59:LEU:HG	1:A:80:LYS:HA	1.91	0.53
1:B:8:TYR:OH	3:F:439:GLU:OE1	2.21	0.53
5:H:40:MET:HE3	5:H:42:ILE:HD11	1.89	0.53
1:B:88:ILE:HG22	1:B:133:LEU:HD11	1.90	0.53
3:C:161:LEU:HD13	3:C:548:VAL:HG22	1.91	0.53
2:E:126:GLU:HG3	2:E:128:SER:H	1.71	0.53
2:E:324:ALA:HB2	2:E:400:ASP:HB2	1.90	0.53
8:J:336:ASN:HB3	8:J:341:ALA:HB1	1.89	0.53
8:J:377:ASP:OD2	8:J:388:ARG:NH2	2.31	0.53
6:I:193:ILE:O	6:I:197:LEU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD21	1:B:106:ARG:HB3	1.91	0.53
3:C:9:LEU:O	3:C:13:LYS:HG2	2.09	0.53
7:K:53:GLU:N	7:K:53:GLU:OE1	2.42	0.53
8:J:114:VAL:HG12	8:J:128:ILE:HB	1.90	0.53
2:E:146:PHE:O	2:E:148:ILE:HG12	2.09	0.53
3:F:26:LYS:O	3:F:59:LEU:N	2.41	0.53
1:A:90:PHE:HE2	1:A:141:LEU:HD23	1.74	0.52
2:E:95:VAL:O	2:D:31:TYR:OH	2.26	0.52
2:D:93:LEU:HD13	2:D:116:VAL:HG12	1.91	0.52
2:D:99:ASP:HB2	2:D:117:PRO:HB3	1.91	0.52
1:B:240:ARG:NH1	2:E:284:ASP:OD2	2.31	0.52
3:C:143:SER:O	3:C:234:GLN:NE2	2.37	0.52
7:K:61:GLN:N	7:K:61:GLN:OE1	2.42	0.52
7:K:216:VAL:HG12	7:K:217:ILE:HD13	1.91	0.52
3:C:385:LEU:HD21	3:C:437:HIS:CD2	2.44	0.52
7:K:235:GLU:HG3	7:K:236:LEU:HD23	1.92	0.52
8:J:23:TYR:CE2	8:J:304:LYS:HE3	2.44	0.52
8:J:197:THR:HG23	8:J:198:TYR:HD1	1.74	0.52
1:A:22:LEU:HD21	1:A:106:ARG:HB3	1.92	0.52
2:D:435:GLY:O	2:D:438:SER:OG	2.28	0.52
8:J:111:TRP:CE3	8:J:155:LEU:HD21	2.44	0.52
8:J:324:PHE:HB2	8:J:331:LEU:HD11	1.90	0.52
3:C:553:LYS:HG2	4:G:4:ILE:HD12	1.90	0.52
12:C:602:COM:H22	13:F:602:F43:C6B	2.40	0.52
3:F:144:LEU:HA	3:F:234:GLN:HG3	1.91	0.52
7:K:1:MET:O	7:K:28:GLU:N	2.42	0.52
7:K:277:LYS:HZ2	7:K:311:LYS:HB2	1.74	0.52
2:E:367:TYR:HE2	10:E:601:SHT:HCC1	1.75	0.52
5:H:232:GLU:N	5:H:232:GLU:OE2	2.43	0.52
7:K:31:VAL:HG22	7:K:217:ILE:HD11	1.91	0.52
7:K:348:ASP:OD1	7:K:348:ASP:N	2.42	0.52
8:J:32:ILE:HD13	8:J:194:LYS:O	2.10	0.52
8:J:256:THR:HG22	8:J:282:VAL:HG12	1.91	0.52
1:B:188:VAL:HG23	1:B:208:PRO:HD3	1.92	0.52
5:H:212:TYR:CD2	8:J:149:ILE:HB	2.45	0.52
7:K:310:GLU:O	7:K:481:THR:OG1	2.23	0.52
7:K:472:GLN:HE21	7:K:495:VAL:HA	1.74	0.52
8:J:41:LYS:O	8:J:172:GLU:HB3	2.10	0.52
1:B:138:LYS:NZ	1:B:143:ASP:OD2	2.42	0.51
2:D:298:ASP:HB3	2:D:301:LYS:HB2	1.92	0.51
7:K:6:VAL:HG21	7:K:24:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:76:GLU:O	7:K:189:VAL:HG11	2.10	0.51
8:J:478:VAL:HG11	8:J:498:VAL:HG21	1.92	0.51
1:A:39:VAL:O	1:A:43:MET:HG3	2.11	0.51
2:D:27:ILE:HA	2:D:32:ASN:HD22	1.76	0.51
5:H:80:LEU:HD22	5:H:85:LEU:HD13	1.91	0.51
5:H:209:GLU:HG3	8:J:149:ILE:HD11	1.83	0.51
7:K:231:GLU:OE2	7:K:231:GLU:N	2.33	0.51
8:J:70:TRP:HZ3	8:J:127:LEU:HD11	1.75	0.51
8:J:324:PHE:HE2	8:J:360:VAL:HG11	1.75	0.51
1:A:6:GLN:O	1:A:7:PHE:C	2.54	0.51
2:D:49:ASN:HB3	2:D:174:ASN:HB3	1.92	0.51
2:E:117:PRO:HG2	2:E:120:ARG:HG3	1.93	0.51
5:H:128:GLN:HA	5:H:155:ILE:HG13	1.93	0.51
7:K:124:GLY:O	7:K:168:ARG:N	2.43	0.51
3:F:25:THR:O	3:F:29:THR:OG1	2.24	0.51
8:J:238:GLN:HG3	8:J:238:GLN:O	2.10	0.51
2:E:364:HIS:O	3:C:249:GLU:HB3	2.11	0.51
3:C:39:LYS:HE3	3:C:68:LEU:HD23	1.91	0.51
3:C:375:ASP:OD1	3:C:376:VAL:N	2.44	0.51
3:C:481:TYR:O	3:C:488:GLN:NE2	2.40	0.51
8:J:48:LEU:HB3	8:J:168:GLU:HB3	1.92	0.51
8:J:179:TYR:CZ	8:J:295:PHE:CB	2.75	0.51
3:C:40:ARG:O	3:C:44:GLU:HG3	2.11	0.51
2:D:94:LYS:HE3	2:D:97:GLU:O	2.12	0.50
1:B:160:HIS:ND1	13:F:601:F43:OCC	2.39	0.50
3:F:123:ARG:NH1	3:F:254:ASP:OD2	2.42	0.50
3:F:258:ALA:HA	3:F:262:ALA:HB3	1.93	0.50
5:H:44:ILE:HD11	5:H:49:ILE:HD13	1.92	0.50
3:C:230:TRP:HA	3:F:329:GLY:HA3	1.94	0.50
7:K:241:ILE:HD12	7:K:248:MET:HE3	1.93	0.50
5:H:147:LYS:NZ	14:H:401:S5Q:S5A	2.77	0.50
7:K:171:SER:HB3	16:K:603:ATP:H2'	1.93	0.50
7:K:277:LYS:NZ	7:K:311:LYS:HB2	2.26	0.50
8:J:28:SER:HA	8:J:300:HIS:CB	2.42	0.50
8:J:41:LYS:O	8:J:172:GLU:C	2.54	0.50
3:C:150:VAL:HG13	6:I:118:HIS:CE1	2.47	0.50
3:F:229:ARG:O	3:F:233:MET:HG2	2.11	0.50
7:K:69:CYS:HB3	7:K:72:CYS:SG	2.51	0.50
1:A:148:ASP:OD2	1:A:151:THR:OG1	2.22	0.50
3:C:524:ASP:HB3	3:C:531:GLU:OE2	2.12	0.50
5:H:32:HIS:ND1	5:H:34:MET:HE3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:17:GLU:HG2	7:K:20:LYS:HD2	1.92	0.50
5:H:222:LEU:HD22	5:H:291:LEU:HD21	1.93	0.50
8:J:111:TRP:HA	8:J:130:VAL:O	2.11	0.50
2:E:214:PHE:HB2	2:E:428:PRO:HG2	1.94	0.50
2:D:357:VAL:CG1	3:C:448:GL3:HA2	2.37	0.50
5:H:208:MET:HA	5:H:208:MET:HE2	1.93	0.50
1:A:184:LYS:HD2	1:A:185:THR:HG23	1.93	0.49
3:F:13:LYS:O	3:F:17:GLU:HB2	2.12	0.49
8:J:46:LYS:O	8:J:46:LYS:HG2	2.12	0.49
2:E:310:LEU:HD11	2:E:331:ILE:HA	1.93	0.49
2:D:95:VAL:HG23	2:D:117:PRO:HG2	1.93	0.49
3:C:311:VAL:HG23	3:C:493:GLY:HA3	1.94	0.49
3:F:194:GLU:OE2	3:F:194:GLU:N	2.29	0.49
8:J:66:THR:HB	8:J:145:ILE:HB	1.95	0.49
3:C:552:ALA:O	4:G:2:ALA:N	2.46	0.49
5:H:77:SER:OG	5:H:79:SER:O	2.30	0.49
5:H:212:TYR:OH	8:J:59:GLY:HA3	2.11	0.49
8:J:291:GLU:CD	8:J:291:GLU:H	2.19	0.49
1:B:137:SER:HA	1:B:141:LEU:HB2	1.93	0.49
3:C:328:SER:HB3	11:C:601:TP7:H52C	1.95	0.49
6:I:127:LEU:HD22	6:I:166:GLY:HA3	1.93	0.49
3:C:98:ILE:HG22	3:C:321:ILE:HD11	1.95	0.49
3:C:447:TYR:HB3	3:C:448:GL3:N	2.27	0.49
6:I:45:PRO:HA	6:I:50:ILE:HG13	1.95	0.49
1:A:133:LEU:HA	1:A:136:PHE:CE2	2.48	0.49
6:I:112:PHE:HB3	6:I:119:ILE:HG12	1.94	0.49
2:D:139:LYS:HD3	2:D:157:HIS:HB2	1.95	0.49
3:F:26:LYS:HG2	3:F:59:LEU:HB3	1.94	0.49
2:E:118:THR:O	2:E:122:GLU:HG2	2.13	0.49
2:E:367:TYR:OH	13:F:601:F43:H4A	2.13	0.49
3:F:311:VAL:HG23	3:F:493:GLY:HA3	1.94	0.49
7:K:64:TYR:O	7:K:96:VAL:N	2.41	0.49
2:D:361:PHE:HB2	3:C:448:GL3:HA1	1.95	0.48
8:J:23:TYR:HE2	8:J:304:LYS:HB2	1.77	0.48
2:E:162:GLY:O	2:E:163:ASN:HB2	2.14	0.48
2:D:324:ALA:HB2	2:D:400:ASP:HB2	1.95	0.48
8:J:92:PHE:HB2	8:J:127:LEU:HB3	1.95	0.48
8:J:91:SER:HA	8:J:128:ILE:HA	1.94	0.48
2:E:139:LYS:HD3	2:E:157:HIS:HB2	1.94	0.48
7:K:124:GLY:O	7:K:168:ARG:HB2	2.13	0.48
2:D:2:VAL:N	2:D:25:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:335:GLN:HG3	13:F:602:F43:OCD	2.12	0.48
8:J:30:ILE:HG23	8:J:195:ILE:HD11	1.95	0.48
8:J:31:VAL:HG21	8:J:292:ILE:HA	1.96	0.48
8:J:93:GLY:HA3	8:J:94:SER:HA	1.57	0.48
2:D:50:LEU:HD22	2:D:78:ALA:HB1	1.94	0.48
2:D:212:ILE:HG22	2:D:245:GLY:HA2	1.95	0.48
6:I:35:ARG:HG2	6:I:37:ASP:OD1	2.14	0.48
3:F:10:LYS:O	3:F:14:GLU:HG3	2.14	0.48
3:F:467:GLU:O	3:F:478:TYR:OH	2.26	0.48
6:I:52:LYS:O	6:I:56:GLU:HG3	2.14	0.48
7:K:380:HIS:H	7:K:380:HIS:CD2	2.30	0.48
8:J:46:LYS:HG3	8:J:57:VAL:HG12	1.95	0.48
7:K:272:GLU:OE2	7:K:272:GLU:N	2.43	0.47
8:J:112:ASP:H	8:J:130:VAL:HB	1.79	0.47
3:C:212:SER:OG	3:C:231:SER:OG	2.27	0.47
5:H:96:VAL:HG13	5:H:101:ALA:HB3	1.97	0.47
8:J:68:ASP:OD1	8:J:68:ASP:N	2.45	0.47
8:J:117:VAL:HA	8:J:125:GLY:CA	2.29	0.47
2:E:286:THR:HA	2:E:292:ASN:HA	1.94	0.47
5:H:126:LEU:HD21	6:I:9:ILE:HG12	1.97	0.47
7:K:193:ALA:HB1	7:K:196:PRO:HB3	1.97	0.47
7:K:316:LEU:HD21	7:K:327:LEU:HD23	1.96	0.47
8:J:109:LYS:HA	8:J:109:LYS:HD3	1.47	0.47
8:J:158:LEU:HD23	8:J:162:ASP:HB2	1.95	0.47
7:K:84:LYS:HD2	7:K:84:LYS:HA	1.59	0.47
1:A:74:GLU:O	1:A:113:ARG:NH2	2.41	0.47
1:A:200:ASP:OD1	1:A:200:ASP:N	2.43	0.47
2:D:351:ARG:HA	3:C:455:SMC:SG	2.55	0.47
7:K:343:GLU:HB3	7:K:350:TRP:HE3	1.79	0.47
8:J:13:LYS:HA	8:J:189:ILE:HG22	1.97	0.47
1:A:89:GLN:NE2	1:A:123:ARG:HD3	2.29	0.47
2:E:236:GLN:HG3	2:E:237:HIS:N	2.29	0.47
3:C:38:ARG:HA	3:C:38:ARG:HD3	1.63	0.47
4:G:22:GLN:O	4:G:26:GLU:HG3	2.15	0.47
3:F:102:TRP:CZ2	3:F:282:PRO:HD3	2.50	0.47
6:I:80:PRO:HB3	6:I:125:LEU:HD13	1.97	0.47
6:I:124:ARG:HB2	6:I:152:ILE:HD11	1.96	0.47
7:K:127:THR:HA	7:K:166:ILE:HA	1.95	0.47
3:C:402:SER:C	3:C:403:MGN:H2	2.23	0.47
5:H:85:LEU:HD21	6:I:62:ARG:HH11	1.80	0.47
8:J:82:LEU:HD11	8:J:90:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:LEU:HD22	2:D:433:ILE:HD12	1.97	0.47
2:E:327:VAL:HG11	2:E:393:VAL:HA	1.97	0.47
3:F:310:VAL:HG21	3:F:496:GLN:HG2	1.96	0.47
3:F:370:MET:O	3:F:374:GLU:HG2	2.14	0.47
7:K:417:GLU:OE2	7:K:417:GLU:N	2.48	0.47
8:J:92:PHE:HZ	8:J:158:LEU:HD22	1.79	0.47
3:C:149:VAL:O	3:C:151:GLN:NE2	2.41	0.46
2:E:362:PHE:HD2	2:E:375:PHE:HE1	1.63	0.46
3:C:102:TRP:CZ2	3:C:282:PRO:HD3	2.50	0.46
3:F:63:ASP:OD2	6:I:129:TYR:OH	2.33	0.46
7:K:95:SER:O	7:K:95:SER:OG	2.29	0.46
2:E:10:LEU:HD13	2:E:433:ILE:HD12	1.96	0.46
2:D:65:LYS:HE3	2:D:65:LYS:HB2	1.56	0.46
7:K:489:MET:O	7:K:493:LEU:HD22	2.15	0.46
8:J:217:LEU:HD21	8:J:222:LEU:HD13	1.97	0.46
1:B:51:ASP:HA	7:K:376:SER:HB3	1.97	0.46
8:J:141:GLU:H	8:J:141:GLU:HG3	1.46	0.46
9:L:28:LYS:HB3	9:L:40:LEU:HD12	1.98	0.46
1:B:202:PRO:HD3	7:K:358:PRO:HG3	1.98	0.46
2:E:125:ALA:HA	2:D:43:LYS:HD3	1.97	0.46
7:K:269:LYS:HE3	7:K:271:PHE:CE1	2.50	0.46
8:J:33:ILE:CD1	8:J:196:TYR:OH	2.64	0.46
8:J:433:ILE:HD12	8:J:462:GLY:HA2	1.98	0.46
2:D:310:LEU:HD11	2:D:331:ILE:HA	1.98	0.46
8:J:15:LEU:O	8:J:16:GLU:C	2.59	0.46
8:J:44:THR:O	8:J:45:LYS:C	2.58	0.46
8:J:99:LEU:HD12	8:J:99:LEU:HA	1.73	0.46
7:K:149:TRP:HA	7:K:152:ASN:ND2	2.31	0.46
8:J:11:SER:O	8:J:12:GLY:C	2.59	0.46
8:J:343:ILE:HG23	8:J:362:THR:HG23	1.98	0.46
2:E:384:HIS:HE2	3:F:483:MET:HE1	1.80	0.46
3:C:282:PRO:HG2	3:C:322:TRP:HE3	1.81	0.46
7:K:515:GLU:HA	7:K:518:LYS:HE2	1.97	0.46
8:J:5:VAL:O	8:J:7:ASN:N	2.49	0.46
8:J:80:LYS:HD2	8:J:80:LYS:HA	1.64	0.46
1:A:161:GLY:HA2	1:A:164:LEU:HG	1.98	0.46
4:G:6:VAL:HG23	4:G:18:GLU:HG3	1.98	0.46
3:F:10:LYS:NZ	3:F:10:LYS:HB3	2.29	0.46
1:A:119:THR:C	1:A:120:LEU:HG	2.41	0.46
2:E:358:GLY:HA2	2:E:361:PHE:CE2	2.51	0.46
2:D:327:VAL:HG11	2:D:393:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:GLN:O	3:C:526:SER:HA	2.15	0.46
6:I:49:HIS:O	6:I:53:PRO:HD2	2.15	0.46
8:J:63:GLU:O	8:J:64:ASN:C	2.59	0.46
8:J:113:VAL:HG22	8:J:148:LEU:HD22	1.97	0.46
1:A:113:ARG:HG2	2:D:263:THR:HG22	1.97	0.45
5:H:236:ILE:HG22	5:H:238:ALA:H	1.81	0.45
6:I:127:LEU:HD11	6:I:168:ILE:HG13	1.97	0.45
7:K:474:SER:OG	7:K:480:GLN:OE1	2.33	0.45
8:J:60:ILE:HB	8:J:67:VAL:HG22	1.98	0.45
8:J:103:SER:O	8:J:104:VAL:C	2.59	0.45
1:A:119:THR:O	1:A:120:LEU:HG	2.16	0.45
3:C:101:LEU:HD11	3:C:313:THR:HG23	1.98	0.45
3:C:325:ALA:O	3:F:226:THR:HG23	2.16	0.45
3:F:73:LEU:HD13	6:I:45:PRO:HG2	1.97	0.45
8:J:79:ASP:HB3	8:J:163:ARG:HH12	1.82	0.45
8:J:447:TYR:HB3	8:J:450:TYR:HD2	1.81	0.45
5:H:212:TYR:CE1	8:J:46:LYS:HB2	2.52	0.45
8:J:42:GLU:HB2	8:J:172:GLU:H	1.80	0.45
2:E:416:GLY:O	2:E:420:SER:OG	2.29	0.45
8:J:311:SER:O	8:J:311:SER:OG	2.33	0.45
2:E:110:LYS:HB3	2:E:110:LYS:HE2	1.74	0.45
6:I:145:GLU:HB2	6:I:157:VAL:HG21	1.97	0.45
8:J:121:ASP:HB2	8:J:124:GLU:HB2	1.99	0.45
3:F:444:LEU:HD23	3:F:450:ASP:HB3	1.98	0.45
8:J:28:SER:HA	8:J:300:HIS:HB2	1.98	0.45
2:D:324:ALA:O	2:D:372:PRO:HG3	2.16	0.45
2:D:354:GLY:HA3	3:C:455:SMC:HCS3	1.99	0.45
7:K:103:GLU:O	7:K:104:ILE:HD13	2.16	0.45
7:K:112:ILE:HG22	7:K:190:ILE:HG22	1.99	0.45
1:B:189:MET:HE3	1:B:189:MET:HB3	1.80	0.45
3:C:88:ASP:HA	3:F:155:VAL:HB	1.99	0.45
3:C:216:SER:O	3:C:220:ARG:HG2	2.16	0.45
3:C:335:GLN:N	13:F:602:F43:OBD	2.50	0.45
3:F:151:GLN:O	3:F:154:MET:HG2	2.17	0.45
8:J:85:LYS:HB2	8:J:85:LYS:HE3	1.74	0.45
2:E:423:ASP:HB3	2:E:431:TYR:CE2	2.52	0.44
3:C:403:MGN:O	3:C:404:ARG:N	2.49	0.44
3:F:195:GLU:H	3:F:195:GLU:CD	2.23	0.44
8:J:87:ILE:H	8:J:87:ILE:HG13	1.45	0.44
1:A:184:LYS:HD2	1:A:185:THR:CG2	2.47	0.44
2:E:167:VAL:HG22	3:C:269:ASN:CG	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:THR:HG23	3:F:325:ALA:O	2.18	0.44
3:F:110:ILE:HB	3:F:265:ILE:HB	1.99	0.44
7:K:19:LEU:HD22	7:K:22:VAL:HG21	1.99	0.44
7:K:35:LEU:HD13	7:K:233:ILE:HG13	1.99	0.44
2:D:351:ARG:HG2	3:C:455:SMC:SG	2.57	0.44
3:C:320:GLN:OE1	3:C:341:TYR:OH	2.34	0.44
3:C:336:TYR:HD1	3:C:403:MGN:HB22	1.83	0.44
7:K:141:TYR:HB3	7:K:145:ASP:HB2	1.99	0.44
8:J:30:ILE:HG23	8:J:195:ILE:CD1	2.46	0.44
8:J:291:GLU:HA	8:J:294:ASP:HB2	2.00	0.44
2:D:366:ILE:HD13	3:F:237:MET:SD	2.58	0.44
7:K:324:LYS:NZ	16:K:603:ATP:O3G	2.50	0.44
8:J:51:THR:HB	8:J:158:LEU:HD21	2.00	0.44
2:D:271:VAL:HG21	2:D:309:GLY:HA3	2.00	0.44
3:F:410:ALA:HB2	3:F:490:GLU:HG2	2.00	0.44
7:K:20:LYS:HG3	7:K:247:GLU:HG3	2.00	0.44
8:J:380:ALA:O	8:J:384:SER:OG	2.24	0.44
2:D:139:LYS:HG3	2:D:160:ILE:HD12	1.99	0.44
5:H:252:LYS:HE2	5:H:283:MET:HE2	1.99	0.44
6:I:144:MET:HG2	6:I:154:THR:CG2	2.47	0.44
7:K:154:ILE:HA	7:K:157:VAL:HG22	1.99	0.44
7:K:313:ILE:HG21	7:K:495:VAL:HG12	2.00	0.44
8:J:48:LEU:HB3	8:J:168:GLU:CB	2.48	0.44
2:D:146:PHE:O	2:D:148:ILE:N	2.51	0.44
3:C:316:ALA:O	3:C:320:GLN:HB2	2.17	0.44
2:E:72:ARG:NH2	2:E:154:SER:OG	2.51	0.44
3:C:447:TYR:N	3:C:448:GL3:N	2.60	0.44
5:H:69:ALA:HB2	5:H:100:GLY:HA3	1.99	0.44
5:H:157:LEU:HD23	5:H:157:LEU:HA	1.84	0.44
8:J:388:ARG:NH1	8:J:497:GLU:OE1	2.37	0.44
3:F:290:LEU:HD21	3:F:314:GLY:HA2	2.00	0.43
7:K:170:LEU:HD23	7:K:170:LEU:HA	1.87	0.43
7:K:173:GLY:O	7:K:177:ARG:HD3	2.18	0.43
7:K:501:LEU:HB2	7:K:516:ILE:HD12	2.00	0.43
8:J:117:VAL:CA	8:J:125:GLY:HA2	2.30	0.43
2:E:310:LEU:HD11	2:E:331:ILE:HG12	2.00	0.43
3:C:446:PHE:O	3:C:449:TYR:HB3	2.17	0.43
7:K:69:CYS:HB2	7:K:74:ASN:H	1.83	0.43
1:B:171:MET:HE2	1:B:171:MET:HB3	1.84	0.43
3:C:101:LEU:HD12	3:C:523:PHE:CZ	2.53	0.43
5:H:185:LYS:HB2	5:H:188:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:77:PHE:HE1	8:J:93:GLY:HA3	1.83	0.43
2:E:99:ASP:OD1	2:E:117:PRO:HB3	2.17	0.43
2:E:271:VAL:HG21	2:E:309:GLY:HA3	1.99	0.43
2:D:10:LEU:HD13	2:D:433:ILE:HG23	1.99	0.43
3:C:256:SER:O	3:C:260:LYS:HG3	2.18	0.43
5:H:74:ALA:HB2	5:H:130:HIS:CG	2.53	0.43
5:H:278:VAL:HG22	5:H:289:ILE:HG12	2.01	0.43
6:I:154:THR:HB	6:I:157:VAL:O	2.19	0.43
8:J:60:ILE:HA	8:J:146:GLY:HA3	2.00	0.43
8:J:108:PHE:HD2	8:J:134:VAL:HG23	1.83	0.43
8:J:153:ARG:H	8:J:153:ARG:HG3	1.43	0.43
2:D:367:TYR:CE2	13:F:602:F43:O7B	2.72	0.43
5:H:206:LYS:HB2	5:H:206:LYS:HE2	1.61	0.43
8:J:404:TYR:HB2	8:J:414:GLU:HG2	2.01	0.43
1:B:211:GLU:O	1:B:215:ARG:HG2	2.18	0.43
2:D:103:VAL:HG13	2:D:114:VAL:HG12	2.00	0.43
7:K:353:MET:O	7:K:354:THR:OG1	2.29	0.43
7:K:398:GLU:HG3	8:J:461:TYR:CD2	2.54	0.43
8:J:97:ILE:HG22	8:J:99:LEU:HB2	1.99	0.43
8:J:168:GLU:HG2	8:J:171:ARG:NH1	2.24	0.43
8:J:376:TYR:OH	8:J:476:LYS:HD3	2.19	0.43
1:A:88:ILE:HG22	1:A:133:LEU:HD11	2.00	0.43
1:A:155:ARG:HB2	1:A:159:VAL:HG12	2.01	0.43
3:C:438:LYS:HB2	3:C:444:LEU:HD22	2.01	0.43
3:F:282:PRO:HB2	3:F:322:TRP:HB2	1.99	0.43
3:F:327:MET:HE3	3:F:327:MET:HB3	1.94	0.43
7:K:150:ALA:O	7:K:154:ILE:HG22	2.19	0.43
2:D:196:PRO:HG2	2:D:199:HIS:CG	2.54	0.43
8:J:5:VAL:HG21	8:J:10:LYS:HB2	1.99	0.43
2:E:184:MET:HG3	3:F:274:ARG:HD3	2.01	0.43
2:D:27:ILE:H	2:D:27:ILE:HG13	1.74	0.43
3:C:275:AGM:O	3:C:276:ALA:C	2.61	0.43
5:H:98:LYS:HB2	5:H:98:LYS:HE2	1.70	0.43
7:K:145:ASP:OD1	7:K:145:ASP:N	2.51	0.43
7:K:462:ILE:HA	7:K:465:ASN:ND2	2.33	0.43
1:A:43:MET:HE3	1:A:45:HIS:CD2	2.54	0.42
2:E:142:LEU:HD12	2:E:160:ILE:HD11	2.00	0.42
7:K:281:LEU:HD22	7:K:308:ILE:HG13	2.00	0.42
8:J:168:GLU:CG	8:J:171:ARG:HH12	2.23	0.42
1:A:8:TYR:OH	3:C:439:GLU:OE1	2.26	0.42
1:A:121:SER:OG	13:F:602:F43:O7C	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:THR:O	2:D:122:GLU:HG2	2.17	0.42
3:C:137:MET:HA	3:C:140:ILE:HG22	2.02	0.42
8:J:41:LYS:O	8:J:172:GLU:CB	2.67	0.42
8:J:241:PHE:CD1	8:J:241:PHE:C	2.97	0.42
2:D:361:PHE:HA	3:C:447:TYR:HB3	1.99	0.42
8:J:32:ILE:HD13	8:J:195:ILE:HA	2.01	0.42
1:A:204:ASP:OD1	1:A:206:GLY:N	2.52	0.42
1:B:90:PHE:HE2	1:B:141:LEU:HD23	1.84	0.42
2:D:384:HIS:CD2	3:C:451:LEU:HD11	2.55	0.42
6:I:56:GLU:OE2	6:I:59:TYR:OH	2.21	0.42
6:I:143:ASP:OD2	6:I:145:GLU:HB3	2.19	0.42
7:K:327:LEU:O	7:K:331:ILE:HG12	2.19	0.42
8:J:434:ASP:OD1	8:J:434:ASP:N	2.31	0.42
2:E:193:ARG:O	2:E:378:ASN:HB2	2.19	0.42
3:C:66:VAL:N	3:F:149:VAL:O	2.49	0.42
4:G:14:LYS:HB3	4:G:14:LYS:HE2	1.68	0.42
3:F:101:LEU:HD12	3:F:523:PHE:CZ	2.55	0.42
7:K:269:LYS:HD2	7:K:269:LYS:O	2.20	0.42
8:J:75:LYS:O	8:J:78:GLU:HB2	2.20	0.42
1:B:242:HIS:HB2	3:F:435:ILE:HD11	2.01	0.42
3:F:24:TYR:HB3	3:F:27:PHE:HD2	1.84	0.42
3:F:311:VAL:CG2	3:F:493:GLY:HA3	2.50	0.42
8:J:111:TRP:HE3	8:J:155:LEU:HD21	1.82	0.42
8:J:170:MET:HE3	8:J:170:MET:HB3	1.65	0.42
5:H:30:GLN:HB3	5:H:41:THR:HB	2.02	0.42
6:I:172:ILE:HD13	6:I:189:ILE:HG12	2.02	0.42
8:J:19:ILE:HA	8:J:22:GLU:HB2	2.01	0.42
8:J:72:LYS:HZ2	8:J:72:LYS:H	1.67	0.42
8:J:325:GLU:OE1	8:J:325:GLU:HA	2.19	0.42
8:J:448:LYS:HE2	8:J:448:LYS:HB3	1.89	0.42
1:A:141:LEU:O	1:A:147:PHE:HB2	2.20	0.42
1:A:242:HIS:NE2	3:C:428:ASN:OD1	2.49	0.42
3:C:344:ASP:OD1	3:C:344:ASP:N	2.53	0.42
3:C:385:LEU:HD23	3:C:385:LEU:HA	1.82	0.42
3:F:385:LEU:HD21	3:F:437:HIS:CD2	2.55	0.42
13:F:602:F43:H9A3	13:F:602:F43:HAA1	1.81	0.42
5:H:97:ARG:HD3	6:I:13:ARG:O	2.20	0.42
7:K:84:LYS:NZ	7:K:87:CYS:O	2.50	0.42
7:K:411:VAL:HG21	7:K:440:ALA:HB2	2.01	0.42
1:B:53:LYS:HB2	1:B:84:ARG:HD3	2.00	0.42
2:D:429:MET:O	2:D:433:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:76:GLU:HB3	7:K:80:GLN:HG3	2.00	0.42
9:L:40:LEU:HD13	9:L:41:LEU:O	2.20	0.42
3:F:170:PHE:HB3	3:F:186:ILE:HB	2.02	0.42
3:C:54:ARG:O	3:C:57:ILE:HG12	2.20	0.41
3:C:165:CYS:SG	3:C:215:PRO:HD3	2.59	0.41
5:H:239:PRO:HG2	6:I:11:ASP:HB3	2.02	0.41
8:J:170:MET:O	8:J:171:ARG:C	2.63	0.41
2:D:214:PHE:HB2	2:D:428:PRO:HG2	2.01	0.41
3:C:444:LEU:HD12	3:C:444:LEU:HA	1.74	0.41
3:F:187:ASP:HB3	3:F:190:LYS:HB2	2.02	0.41
7:K:258:VAL:HG22	7:K:262:MET:SD	2.61	0.41
2:D:110:LYS:HE2	2:D:110:LYS:HB2	1.76	0.41
3:C:245:LEU:H	3:C:245:LEU:HG	1.72	0.41
3:C:383:TYR:O	3:C:386:GLU:HG2	2.20	0.41
7:K:273:LYS:HD3	7:K:273:LYS:HA	1.70	0.41
1:B:138:LYS:HE3	7:K:385:TYR:OH	2.20	0.41
2:D:167:VAL:HG22	3:F:269:ASN:CG	2.45	0.41
2:D:195:ILE:HD12	2:D:218:MET:HG3	2.01	0.41
3:C:15:LYS:HB3	3:C:15:LYS:HE3	1.97	0.41
3:C:213:ARG:HH21	3:C:518:ASP:HB3	1.84	0.41
3:F:236:GLY:O	3:F:240:ILE:HG23	2.20	0.41
6:I:37:ASP:OD1	6:I:37:ASP:N	2.52	0.41
7:K:33:GLY:HA2	7:K:225:ILE:O	2.20	0.41
7:K:472:GLN:NE2	7:K:495:VAL:HA	2.35	0.41
8:J:121:ASP:O	8:J:122:THR:C	2.62	0.41
2:E:360:SER:O	2:E:364:HIS:HB2	2.21	0.41
8:J:31:VAL:HG11	8:J:292:ILE:HA	2.03	0.41
1:B:250:TYR:O	1:B:251:ILE:HG13	2.20	0.41
3:C:282:PRO:HG2	3:C:322:TRP:CE3	2.56	0.41
3:C:403:MGN:HN21	13:F:602:F43:H6D2	1.84	0.41
1:A:164:LEU:HD22	3:C:396:GLU:HG3	2.03	0.41
2:D:59:ALA:HB3	2:D:61:LYS:HG2	2.03	0.41
2:D:314:VAL:HA	2:D:330:VAL:HG11	2.03	0.41
3:C:7:LEU:HB2	3:C:348:ASP:HB2	2.03	0.41
3:C:446:PHE:CD2	3:C:449:TYR:HB2	2.55	0.41
3:F:282:PRO:HG2	3:F:322:TRP:HE3	1.85	0.41
3:F:316:ALA:O	3:F:320:GLN:HB2	2.21	0.41
5:H:212:TYR:HD2	8:J:149:ILE:HB	1.84	0.41
5:H:272:LEU:HD21	5:H:289:ILE:HD13	2.02	0.41
6:I:120:ILE:HA	6:I:147:PHE:CE1	2.56	0.41
8:J:439:ALA:HB1	8:J:471:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:CD1	1:A:136:PHE:C	2.98	0.41
3:C:169:ILE:HG22	3:C:184:PHE:O	2.20	0.41
3:C:410:ALA:HB2	3:C:490:GLU:HG2	2.03	0.41
4:G:148:LYS:HB2	4:G:148:LYS:HE3	1.94	0.41
3:F:418:MET:HA	3:F:501:ALA:HB2	2.03	0.41
5:H:196:ILE:HD13	5:H:196:ILE:HA	1.85	0.41
6:I:34:LEU:HB3	6:I:35:ARG:H	1.70	0.41
7:K:214:GLU:O	7:K:218:LYS:HB2	2.21	0.41
8:J:50:LYS:HD2	8:J:50:LYS:HA	1.41	0.41
8:J:69:PHE:O	8:J:70:TRP:C	2.63	0.41
8:J:81:SER:HA	8:J:163:ARG:CA	2.47	0.41
8:J:83:ILE:HD13	8:J:83:ILE:HA	1.88	0.41
8:J:131:GLN:HB2	8:J:132:ARG:HH11	1.86	0.41
8:J:260:ILE:HD12	8:J:260:ILE:HA	1.97	0.41
8:J:369:LYS:HE2	8:J:369:LYS:HB2	1.84	0.41
8:J:410:ILE:HD11	8:J:454:ARG:NH2	2.36	0.41
8:J:458:ASN:OD1	8:J:458:ASN:N	2.53	0.41
9:L:14:SER:OG	9:L:15:TYR:N	2.53	0.41
1:A:121:SER:HB3	3:C:444:LEU:O	2.21	0.41
1:A:195:VAL:HG11	3:F:244:LYS:HB3	2.03	0.41
2:D:357:VAL:HG11	3:C:450:ASP:CG	2.46	0.41
3:C:19:ASP:OD1	3:C:20:PRO:HD2	2.21	0.41
3:C:547:ASP:OD1	4:G:32:LYS:HG2	2.21	0.41
3:F:281:GLU:HA	3:F:281:GLU:OE1	2.21	0.41
7:K:22:VAL:HA	7:K:248:MET:SD	2.61	0.41
7:K:422:LEU:HD23	7:K:422:LEU:HA	1.88	0.41
8:J:110:LYS:HD3	8:J:111:TRP:NE1	2.35	0.41
8:J:324:PHE:CD2	8:J:331:LEU:HD21	2.53	0.41
2:D:50:LEU:HD23	2:D:50:LEU:HA	1.91	0.40
3:C:5:LYS:HB2	3:C:5:LYS:HE2	1.82	0.40
6:I:82:ASP:C	6:I:82:ASP:OD1	2.64	0.40
7:K:176:GLN:NE2	7:K:196:PRO:O	2.53	0.40
8:J:111:TRP:CE3	8:J:131:GLN:HA	2.56	0.40
1:A:150:ALA:HB2	1:A:208:PRO:HB3	2.02	0.40
2:E:362:PHE:HD1	10:E:601:SHT:O2P	2.04	0.40
3:C:301:GLU:OE1	3:C:301:GLU:N	2.54	0.40
3:C:309:GLU:OE1	3:C:528:PRO:HD2	2.21	0.40
4:G:132:VAL:O	4:G:136:MET:HG2	2.20	0.40
5:H:244:THR:HA	5:H:249:LEU:HD23	2.02	0.40
2:E:219:GLU:O	2:E:223:THR:HG23	2.21	0.40
2:D:143:ILE:HD13	2:D:148:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LYS:HA	3:C:392:PRO:HD2	2.04	0.40
3:C:161:LEU:HD12	3:C:161:LEU:HA	1.96	0.40
5:H:139:ASN:HA	5:H:163:PRO:HD3	2.03	0.40
8:J:64:ASN:CG	8:J:142:ASN:HB3	2.45	0.40
8:J:409:ASP:OD2	8:J:454:ARG:HB2	2.21	0.40
1:A:100:GLN:OE1	3:C:443:ARG:NH1	2.54	0.40
2:D:41:ASN:OD1	2:D:44:ARG:NH1	2.54	0.40
3:F:61:ASN:HB3	3:F:64:ILE:HG12	2.04	0.40
5:H:47:ASN:O	8:J:229:ASN:ND2	2.45	0.40
5:H:181:GLN:HE21	5:H:181:GLN:HB3	1.67	0.40
7:K:254:SER:O	7:K:258:VAL:HG12	2.22	0.40
7:K:419:GLU:C	7:K:419:GLU:OE2	2.65	0.40
8:J:250:ARG:HD2	8:J:270:TYR:CZ	2.56	0.40
1:A:74:GLU:HA	1:A:75:PRO:HD3	1.92	0.40
4:G:52:ILE:HD13	4:G:52:ILE:HA	1.97	0.40
7:K:250:LEU:HD23	7:K:257:VAL:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/260 (99%)	252 (98%)	5 (2%)	0	100	100
1	B	257/260 (99%)	252 (98%)	5 (2%)	0	100	100
2	D	440/443 (99%)	422 (96%)	18 (4%)	0	100	100
2	E	440/443 (99%)	418 (95%)	21 (5%)	1 (0%)	43	54
3	C	541/553 (98%)	511 (94%)	30 (6%)	0	100	100
3	F	511/553 (92%)	488 (96%)	22 (4%)	1 (0%)	43	54
4	G	110/183 (60%)	106 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	H	294/304 (97%)	288 (98%)	6 (2%)	0	100 100
6	I	192/234 (82%)	186 (97%)	6 (3%)	0	100 100
7	K	519/531 (98%)	469 (90%)	46 (9%)	4 (1%)	16 22
8	J	493/501 (98%)	435 (88%)	47 (10%)	11 (2%)	5 5
9	L	45/93 (48%)	45 (100%)	0	0	100 100
All	All	4099/4358 (94%)	3872 (94%)	210 (5%)	17 (0%)	31 39

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	82	ALA
3	F	153	HIS
7	K	76	GLU
7	K	143	GLY
8	J	6	ASN
8	J	71	ASN
8	J	170	MET
8	J	133	ASP
8	J	136	GLU
8	J	165	ILE
7	K	508	ILE
8	J	11	SER
8	J	104	VAL
7	K	310	GLU
8	J	12	GLY
8	J	167	ILE
8	J	117	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	223/224 (100%)	218 (98%)	5 (2%)	45 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	223/224 (100%)	220 (99%)	3 (1%)	61 74
2	D	341/342 (100%)	334 (98%)	7 (2%)	47 63
2	E	341/342 (100%)	334 (98%)	7 (2%)	47 63
3	C	437/439 (100%)	426 (98%)	11 (2%)	42 58
3	F	412/439 (94%)	402 (98%)	10 (2%)	43 59
4	G	104/168 (62%)	103 (99%)	1 (1%)	68 78
5	H	264/271 (97%)	255 (97%)	9 (3%)	32 47
6	I	160/186 (86%)	153 (96%)	7 (4%)	25 37
7	K	449/458 (98%)	412 (92%)	37 (8%)	10 15
8	J	452/454 (100%)	378 (84%)	74 (16%)	2 2
9	L	43/81 (53%)	43 (100%)	0	100 100
All	All	3449/3628 (95%)	3278 (95%)	171 (5%)	23 33

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	A	195	VAL
1	A	203	VAL
1	A	224	ASP
1	A	226	VAL
1	B	203	VAL
1	B	224	ASP
1	B	228	MET
2	E	114	VAL
2	E	121	LEU
2	E	136	MET
2	E	215	SER
2	E	292	ASN
2	E	327	VAL
2	E	365	SER
2	D	65	LYS
2	D	114	VAL
2	D	163	ASN
2	D	230	VAL
2	D	236	GLN
2	D	405	MET
2	D	415	VAL

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Mol	Chain	Res	Type
3	C	78	LEU
3	C	82	ASP
3	C	149	VAL
3	C	239	PHE
3	C	244	LYS
3	C	245	LEU
3	C	260	LYS
3	C	334	THR
3	C	342	THR
3	C	375	ASP
3	C	427	VAL
4	G	45	VAL
3	F	78	LEU
3	F	115	THR
3	F	157	VAL
3	F	214	VAL
3	F	260	LYS
3	F	274	ARG
3	F	342	THR
3	F	427	VAL
3	F	442	SER
3	F	526	SER
5	H	77	SER
5	H	84	HIS
5	H	93	SER
5	H	151	PHE
5	H	166	LEU
5	H	181	GLN
5	H	203	ILE
5	H	220	VAL
5	H	293	SER
6	I	39	VAL
6	I	81	SER
6	I	104	ARG
6	I	144	MET
6	I	145	GLU
6	I	169	VAL
6	I	173	THR
7	K	32	MET
7	K	58	THR
7	K	62	ILE
7	K	66	VAL

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Mol	Chain	Res	Type
7	K	71	HIS
7	K	72	CYS
7	K	76	GLU
7	K	83	LYS
7	K	84	LYS
7	K	86	GLU
7	K	90	GLU
7	K	98	PHE
7	K	145	ASP
7	K	180	LEU
7	K	186	LYS
7	K	197	THR
7	K	217	ILE
7	K	236	LEU
7	K	239	LYS
7	K	269	LYS
7	K	277	LYS
7	K	291	VAL
7	K	308	ILE
7	K	310	GLU
7	K	311	LYS
7	K	312	GLU
7	K	313	ILE
7	K	361	ARG
7	K	387	LEU
7	K	393	LEU
7	K	394	GLU
7	K	411	VAL
7	K	433	GLU
7	K	466	GLN
7	K	486	SER
7	K	493	LEU
7	K	494	ASN
8	J	8	ASN
8	J	11	SER
8	J	13	LYS
8	J	14	THR
8	J	15	LEU
8	J	17	ASP
8	J	20	LYS
8	J	21	ASP
8	J	23	TYR

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Mol	Chain	Res	Type
8	J	44	THR
8	J	45	LYS
8	J	46	LYS
8	J	48	LEU
8	J	49	ILE
8	J	50	LYS
8	J	52	THR
8	J	53	LYS
8	J	57	VAL
8	J	58	VAL
8	J	60	ILE
8	J	65	GLU
8	J	66	THR
8	J	68	ASP
8	J	72	LYS
8	J	75	LYS
8	J	77	PHE
8	J	78	GLU
8	J	80	LYS
8	J	85	LYS
8	J	87	ILE
8	J	88	SER
8	J	90	VAL
8	J	99	LEU
8	J	101	VAL
8	J	105	LYS
8	J	109	LYS
8	J	110	LYS
8	J	113	VAL
8	J	114	VAL
8	J	116	SER
8	J	121	ASP
8	J	124	GLU
8	J	126	ASN
8	J	127	LEU
8	J	128	ILE
8	J	132	ARG
8	J	133	ASP
8	J	134	VAL
8	J	135	LEU
8	J	137	LEU
8	J	141	GLU

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Mol	Chain	Res	Type
8	J	145	ILE
8	J	148	LEU
8	J	153	ARG
8	J	155	LEU
8	J	156	LYS
8	J	161	ASP
8	J	163	ARG
8	J	164	ILE
8	J	165	ILE
8	J	168	GLU
8	J	169	GLN
8	J	170	MET
8	J	171	ARG
8	J	209	SER
8	J	337	ILE
8	J	338	ASP
8	J	339	GLU
8	J	344	VAL
8	J	362	THR
8	J	408	ASP
8	J	434	ASP
8	J	441	THR
8	J	472	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	83	GLN
2	E	107	ASN
2	E	207	ASN
2	D	16	ASN
2	D	68	GLN
2	D	81	ASN
2	D	83	GLN
2	D	107	ASN
2	D	111	GLN
2	D	163	ASN
2	D	174	ASN
2	D	207	ASN
2	D	384	HIS
3	C	196	GLN
3	C	459	ASN

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Mol	Chain	Res	Type
3	C	480	ASN
4	G	177	GLN
3	F	459	ASN
3	F	480	ASN
3	F	509	ASN
5	H	104	ASN
5	H	115	ASN
5	H	175	ASN
5	H	245	GLN
6	I	36	ASN
6	I	85	GLN
6	I	111	HIS
7	K	80	GLN
7	K	228	HIS
7	K	309	ASN
7	K	472	GLN
8	J	64	ASN
8	J	106	GLN
8	J	190	GLN
8	J	306	ASN
9	L	24	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AGM	C	275	3	10,11,12	0.44	0	6,13,15	0.22	0
3	AGM	F	275	3	10,11,12	0.46	0	6,13,15	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MGN	F	403	3	6,9,10	0.80	0	5,12,14	0.94	0
3	SMC	F	455	3	5,6,7	0.68	0	2,6,8	0.96	0
3	SMC	C	455	3	5,6,7	0.69	0	2,6,8	1.23	0
3	MHS	C	261	3	10,11,12	0.64	0	6,14,16	0.68	0
3	GL3	C	448	-	2,3,4	1.78	1 (50%)	1,2,4	0.45	0
3	MHS	F	261	3	10,11,12	0.62	0	6,14,16	2.77	1 (16%)
3	MGN	C	403	-	6,9,10	0.64	0	5,12,14	0.87	0
3	GL3	F	448	3	2,3,4	1.79	1 (50%)	1,2,4	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGM	C	275	3	-	5/10/11/13	-
3	AGM	F	275	3	-	5/10/11/13	-
3	MGN	F	403	3	-	0/7/9/12	-
3	SMC	F	455	3	-	1/3/5/7	-
3	SMC	C	455	3	-	3/3/5/7	-
3	MHS	C	261	3	-	2/5/6/8	0/1/1/1
3	GL3	C	448	-	-	1/1/1/2	-
3	MHS	F	261	3	-	2/5/6/8	0/1/1/1
3	MGN	C	403	-	-	2/7/9/12	-
3	GL3	F	448	3	-	1/1/1/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	448	GL3	C-S	-2.51	1.72	1.80
3	F	448	GL3	C-S	-2.51	1.72	1.80

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	261	MHS	CB-CA-C	-6.69	98.93	111.47

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	261	MHS	O-C-CA-CB
3	C	275	AGM	O-C-CA-CB
3	C	275	AGM	CE2-CD-NE1-CZ
3	C	275	AGM	NH1-CZ-NE1-CD
3	C	275	AGM	NH2-CZ-NE1-CD
3	C	403	MGN	O-C-CA-CB2
3	C	448	GL3	S-C-CA-N
3	C	455	SMC	N-CA-CB-SG
3	C	455	SMC	C-CA-CB-SG
3	C	455	SMC	CA-CB-SG-CS
3	F	261	MHS	O-C-CA-CB
3	F	261	MHS	N-CA-CB-CG
3	F	275	AGM	N-CA-CB-CG
3	F	275	AGM	C-CA-CB-CG
3	F	275	AGM	NH1-CZ-NE1-CD
3	F	275	AGM	NH2-CZ-NE1-CD
3	F	448	GL3	S-C-CA-N
3	F	455	SMC	CA-CB-SG-CS
3	F	275	AGM	CE2-CD-NE1-CZ
3	C	261	MHS	N-CA-CB-CG
3	C	403	MGN	CB2-CA-CB1-CG
3	C	275	AGM	CG-CD-NE1-CZ

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	275	AGM	1	0
3	C	455	SMC	3	0
3	C	261	MHS	1	0
3	C	448	GL3	17	0
3	C	403	MGN	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	F43	F	602	12,3	61,71,71	2.04	4 (6%)	64,118,118	1.11	4 (6%)
13	F43	F	601	-	61,71,71	1.96	4 (6%)	64,118,118	1.02	5 (7%)
14	S5Q	I	201	6	18,30,30	2.58	11 (61%)	-		
11	TP7	C	601	-	19,20,20	1.59	3 (15%)	24,26,26	1.10	2 (8%)
14	S5Q	I	202	6	18,30,30	2.62	12 (66%)	-		
16	ATP	K	602	17	29,33,33	0.29	0	44,52,52	0.47	1 (2%)
16	ATP	K	603	17	29,33,33	0.28	0	44,52,52	0.45	1 (2%)
10	SHT	E	601	-	26,27,27	1.28	2 (7%)	30,36,36	0.74	0
14	S5Q	H	401	5	18,30,30	2.58	12 (66%)	-		
12	COM	C	602	13	6,6,6	0.42	0	7,8,8	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	F43	F	602	12,3	-	14/28/185/185	-
13	F43	F	601	-	-	9/28/185/185	-
11	TP7	C	601	-	-	4/24/24/24	-
16	ATP	K	602	17	-	3/22/38/38	0/3/3/3
16	ATP	K	603	17	-	2/22/38/38	0/3/3/3
10	SHT	E	601	-	-	18/31/31/31	-
12	COM	C	602	13	-	4/4/4/4	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	602	F43	NI-NA	9.77	2.10	1.89
13	F	601	F43	NI-NA	9.36	2.09	1.89
13	F	602	F43	NI-NB	9.19	2.09	1.89
13	F	601	F43	NI-NB	9.12	2.09	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	602	F43	NI-ND	7.18	2.05	1.89
13	F	601	F43	NI-ND	6.83	2.04	1.89
11	C	601	TP7	C1-N	5.20	1.45	1.34
10	E	601	SHT	CK1-CK	-5.17	1.37	1.48
14	I	201	S5Q	S4B-FE7	-4.34	2.21	2.32
14	I	202	S5Q	S4B-FE7	-4.32	2.21	2.32
14	I	202	S5Q	S3B-FE6	-4.29	2.21	2.32
14	H	401	S5Q	S4B-FE7	-4.29	2.21	2.32
14	H	401	S5Q	S3B-FE6	-4.23	2.22	2.32
14	I	201	S5Q	S3B-FE6	-4.23	2.22	2.32
14	I	202	S5Q	S1B-FE6	-3.50	2.23	2.32
14	I	201	S5Q	S1B-FE6	-3.47	2.23	2.32
14	H	401	S5Q	S1B-FE6	-3.42	2.24	2.32
14	I	202	S5Q	S3B-FE7	-3.20	2.24	2.32
14	H	401	S5Q	S2A-FE2	-3.20	2.24	2.32
14	I	202	S5Q	S2A-FE2	-3.16	2.24	2.32
14	I	201	S5Q	S2A-FE2	-3.15	2.24	2.32
14	I	201	S5Q	S3B-FE7	-3.08	2.24	2.32
14	H	401	S5Q	S3B-FE7	-3.04	2.24	2.32
14	H	401	S5Q	S2B-FE6	-3.01	2.17	2.24
11	C	601	TP7	P-O4P	2.99	1.65	1.59
14	I	201	S5Q	S2B-FE6	-2.92	2.18	2.24
14	I	202	S5Q	S2B-FE6	-2.92	2.18	2.24
14	I	201	S5Q	S4A-FE3	-2.90	2.25	2.32
14	H	401	S5Q	S4A-FE3	-2.86	2.25	2.32
14	I	202	S5Q	S4A-FE3	-2.86	2.25	2.32
14	I	202	S5Q	S1B-FE5	-2.68	2.25	2.32
14	I	201	S5Q	S4B-FE5	-2.62	2.25	2.32
14	I	202	S5Q	S4B-FE5	-2.60	2.26	2.32
14	H	401	S5Q	S1B-FE5	-2.59	2.26	2.32
13	F	602	F43	C4C-NC	2.57	1.39	1.35
14	H	401	S5Q	S4B-FE5	-2.54	2.26	2.32
14	I	201	S5Q	S1B-FE5	-2.52	2.26	2.32
13	F	601	F43	C4C-NC	2.50	1.39	1.35
14	H	401	S5Q	S2A-FE3	-2.39	2.26	2.32
14	I	202	S5Q	S2A-FE3	-2.38	2.26	2.32
14	I	201	S5Q	S2A-FE3	-2.36	2.26	2.32
14	I	202	S5Q	S1A-FE2	-2.33	2.26	2.32
14	H	401	S5Q	S1A-FE2	-2.26	2.26	2.32
14	I	201	S5Q	S1A-FE2	-2.26	2.26	2.32
11	C	601	TP7	O1-C1	-2.23	1.18	1.23
10	E	601	SHT	OS2-SG2	2.14	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	401	S5Q	S2B-FE2	-2.06	2.20	2.24
14	I	202	S5Q	S2B-FE2	-2.01	2.20	2.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	602	F43	C2B-C1B-NB	3.47	107.04	101.84
13	F	601	F43	C2A-C3A-C4A	-3.25	97.39	102.36
13	F	602	F43	C3D-C4D-ND	3.20	107.31	102.34
13	F	601	F43	C3D-C4D-ND	3.11	107.18	102.34
13	F	601	F43	C2B-C3B-C4B	-2.73	98.55	101.63
13	F	602	F43	C4B-CHC-C1C	2.71	130.28	125.84
13	F	602	F43	C2A-C3A-C4A	-2.45	98.63	102.36
13	F	601	F43	C9D-C3D-C4D	-2.41	108.31	114.67
11	C	601	TP7	C2-C1-N	2.25	119.74	115.83
13	F	601	F43	C3D-C2D-C1D	2.11	106.25	102.69
11	C	601	TP7	CG-CB-CA	-2.05	109.10	113.17
16	K	603	ATP	PB-O3B-PG	2.03	139.78	132.83
16	K	602	ATP	PB-O3B-PG	2.02	139.76	132.83

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	E	601	SHT	CC-CD-SG2-OS3
10	E	601	SHT	CC-CD-SG2-OS1
10	E	601	SHT	CK1-CK-N-CA
10	E	601	SHT	OK-CK-N-CA
10	E	601	SHT	CB-CA-N-CK
10	E	601	SHT	N-CA-CB-CG2
10	E	601	SHT	N-CA-CB-O3'
10	E	601	SHT	C-CA-CB-CG2
12	C	602	COM	C1-C2-S2-O1S
12	C	602	COM	C1-C2-S2-O2S
12	C	602	COM	C1-C2-S2-O3S
13	F	601	F43	C1A-C2A-C5A-C6A
13	F	601	F43	C9A-C2A-C5A-C6A
13	F	601	F43	C2A-C3A-CAA-CBA
13	F	602	F43	C2A-C3A-CAA-CBA
13	F	602	F43	C4A-C3A-CAA-CBA
16	K	602	ATP	PB-O3B-PG-O3G
10	E	601	SHT	CK3-CK4-CK5-CK6

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Mol	Chain	Res	Type	Atoms
13	F	602	F43	C3C-C8C-C9C-CAC
10	E	601	SHT	O-C-CA-CB
10	E	601	SHT	O-C-CA-N
11	C	601	TP7	C2-C3-C4-C5
16	K	602	ATP	PG-O3B-PB-O1B
10	E	601	SHT	CC-CD-SG2-OS2
13	F	602	F43	C2C-C3C-C8C-C9C
10	E	601	SHT	CK5-CK6-SK-S1
13	F	602	F43	C3C-C2C-C5C-C6C
10	E	601	SHT	OXT-C-CA-CB
13	F	602	F43	C2C-C5C-C6C-O8C
10	E	601	SHT	C-CA-CB-O3'
10	E	601	SHT	OXT-C-CA-N
16	K	603	ATP	PA-O3A-PB-O2B
12	C	602	COM	S1-C1-C2-S2
13	F	601	F43	C4A-C3A-CAA-CBA
13	F	601	F43	C1C-C2C-C5C-C6C
13	F	602	F43	C1C-C2C-C5C-C6C
10	E	601	SHT	OK-CK-CK1-CK2
10	E	601	SHT	N-CK-CK1-CK2
13	F	602	F43	C2C-C5C-C6C-O7C
13	F	601	F43	C2B-C3B-CAB-CBB
11	C	601	TP7	C1-C2-C3-C4
13	F	601	F43	CAB-CBB-CCB-ODB
13	F	602	F43	C4C-C3C-C8C-C9C
13	F	602	F43	C8C-C9C-CAC-OCC
13	F	602	F43	C8C-C9C-CAC-OBC
16	K	602	ATP	PG-O3B-PB-O2B
13	F	602	F43	CAA-CBA-CCA-ODA
11	C	601	TP7	CB-O4P-P-O1P
13	F	601	F43	CAB-CBB-CCB-OEB
13	F	602	F43	CAB-CBB-CCB-ODB
13	F	602	F43	CAA-CBA-CCA-OEA
11	C	601	TP7	CB-O4P-P-O3P
16	K	603	ATP	PA-O3A-PB-O1B
13	F	601	F43	C3A-CAA-CBA-CCA

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	602	F43	10	0

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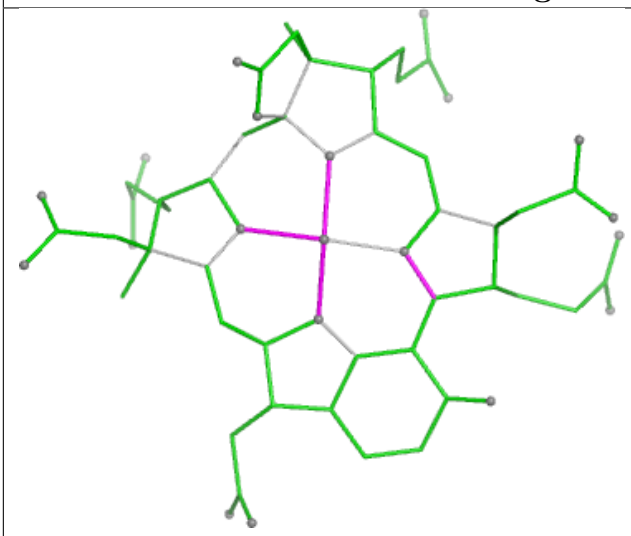
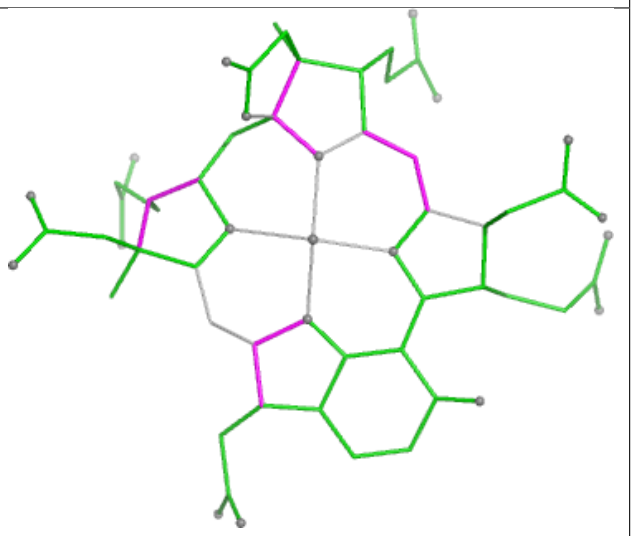
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	601	F43	5	0
11	C	601	TP7	1	0
16	K	603	ATP	2	0
10	E	601	SHT	2	0
14	H	401	S5Q	1	0
12	C	602	COM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

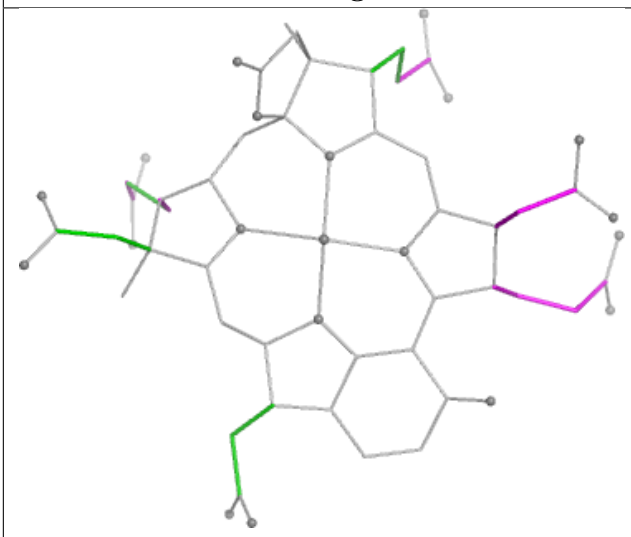
Ligand F43 F 602



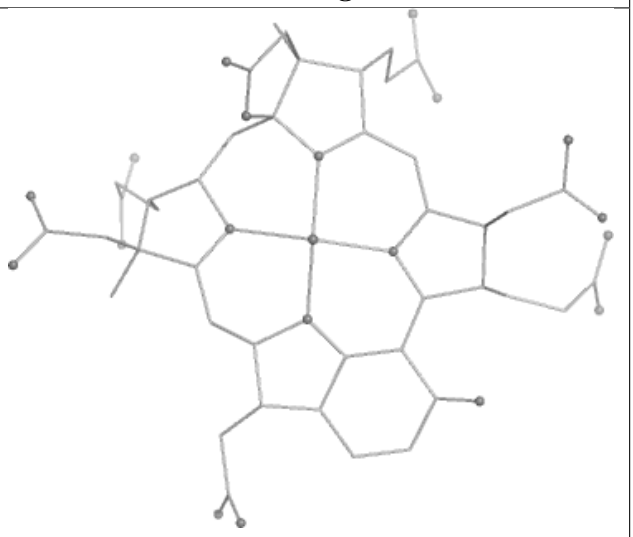
Bond lengths



Bond angles

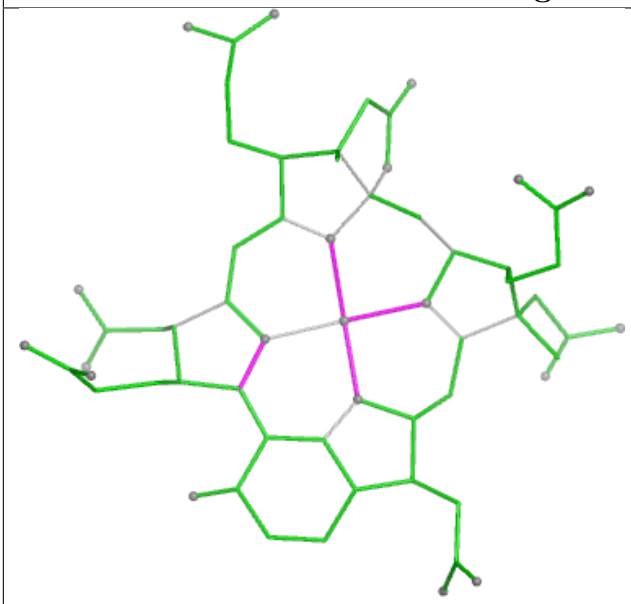


Torsions



Rings

Ligand F43 F 601



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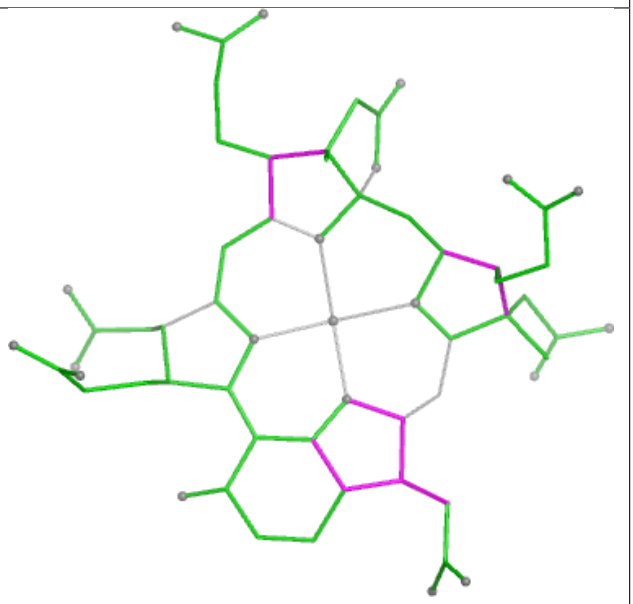

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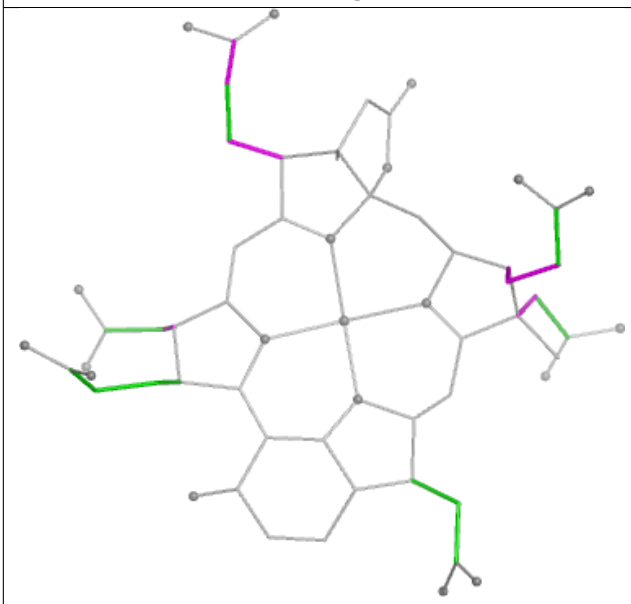
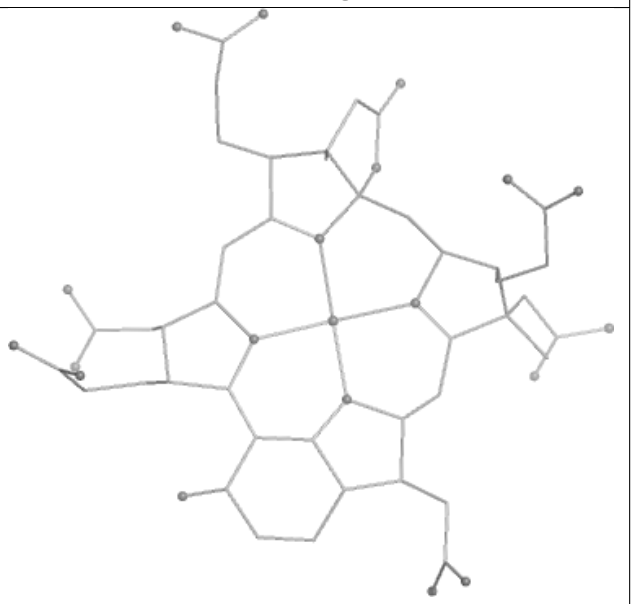
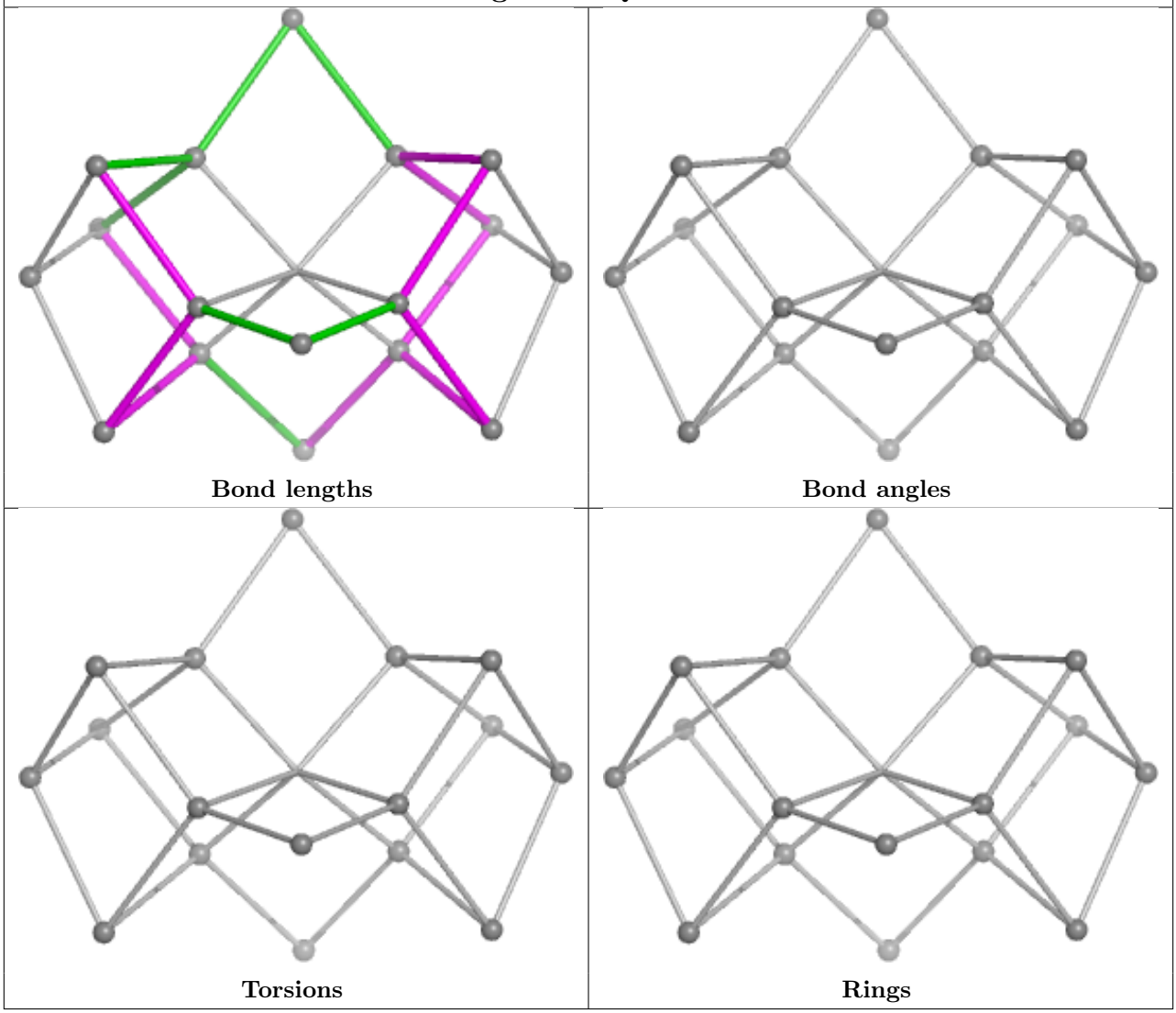


Torsions

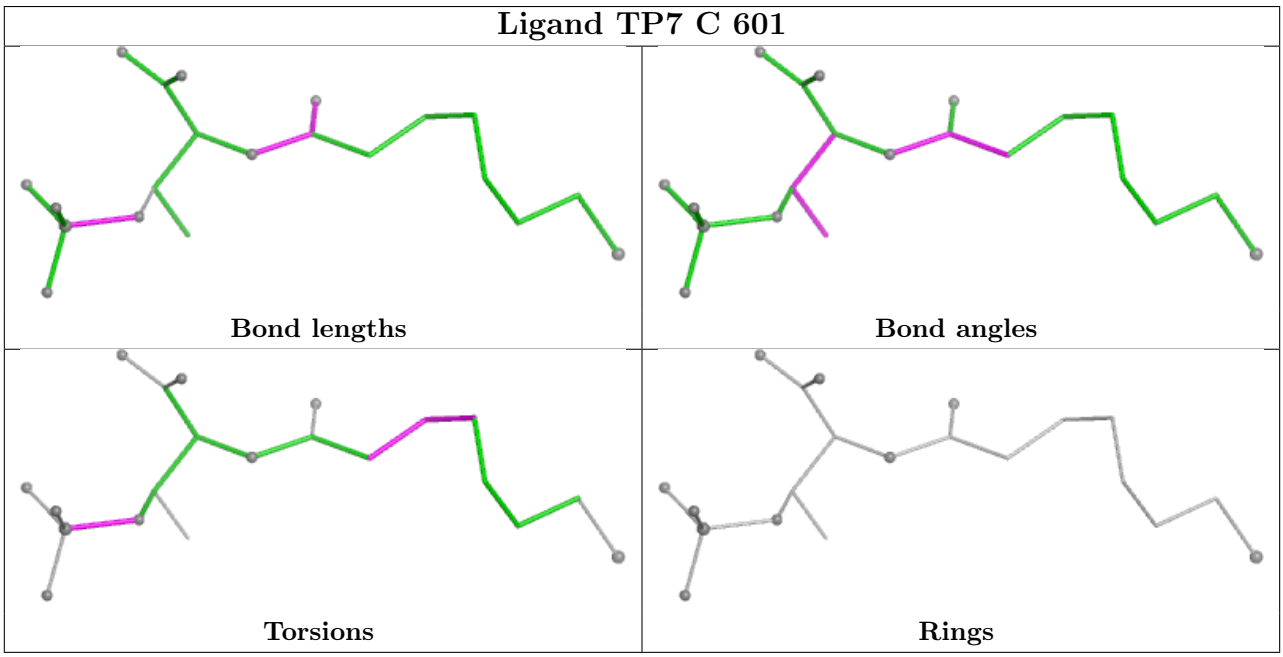


Rings

Ligand S5Q I 201



Ligand TP7 C 601



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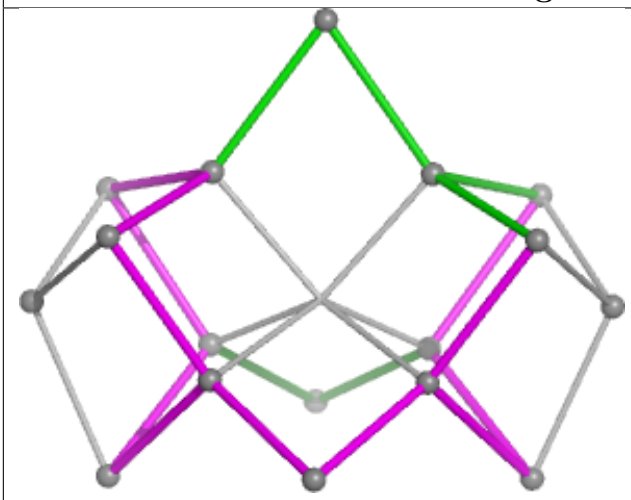

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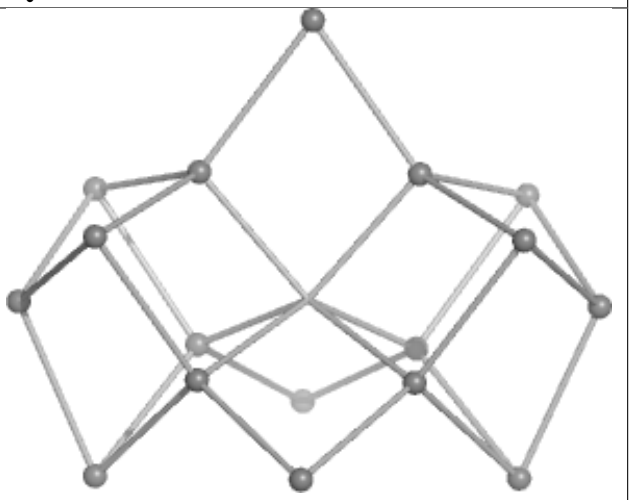
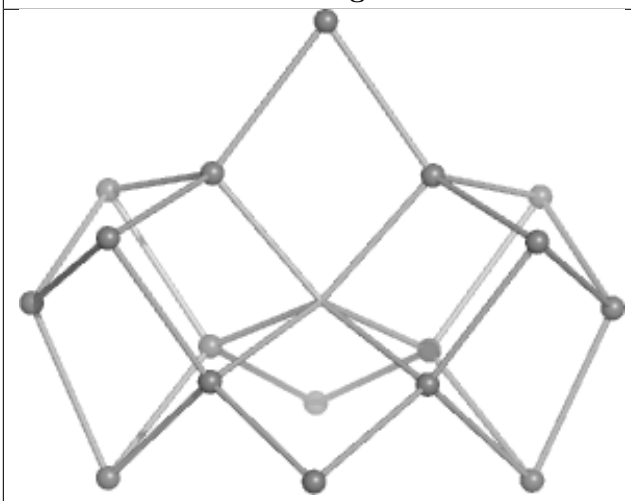


Bond angles



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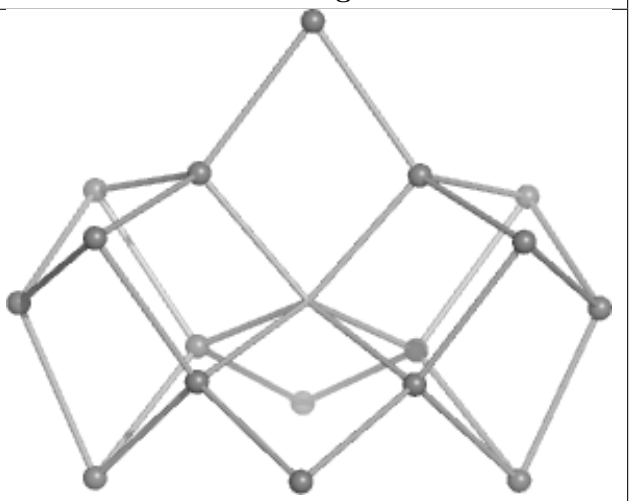
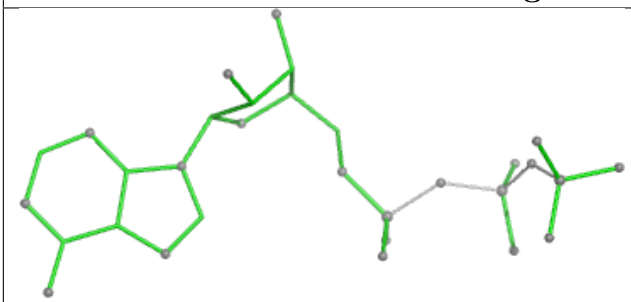


Rings

Ligand ATP K 602



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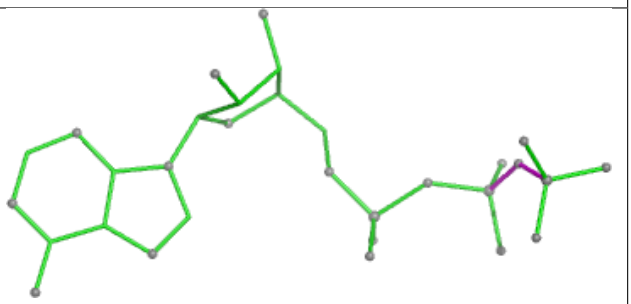
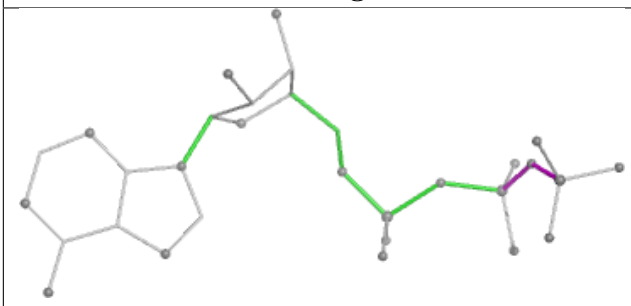


Bond angles



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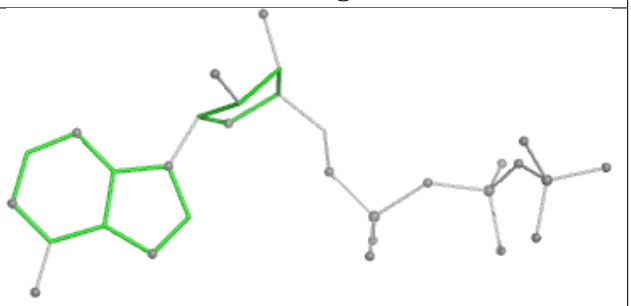

Rings

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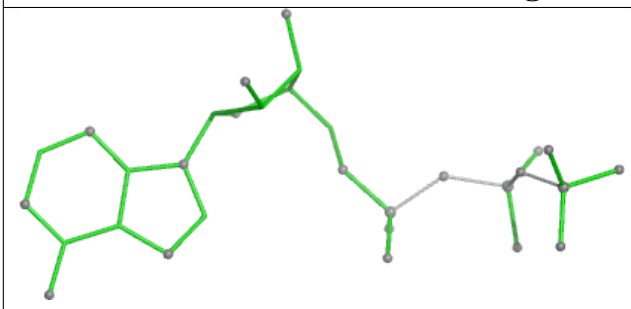

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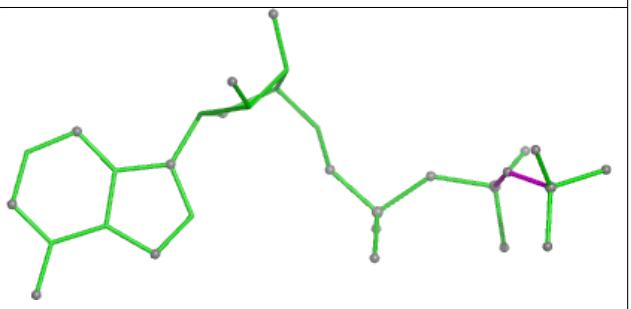
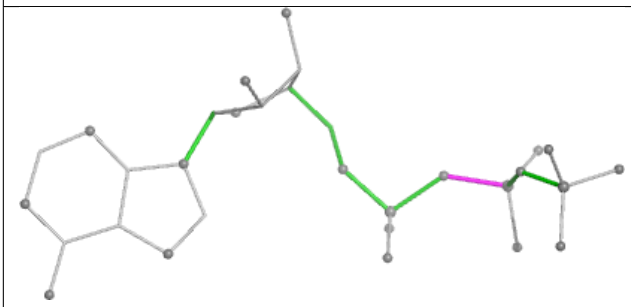


Bond angles



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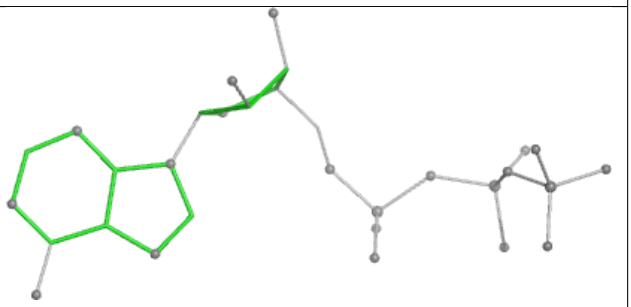
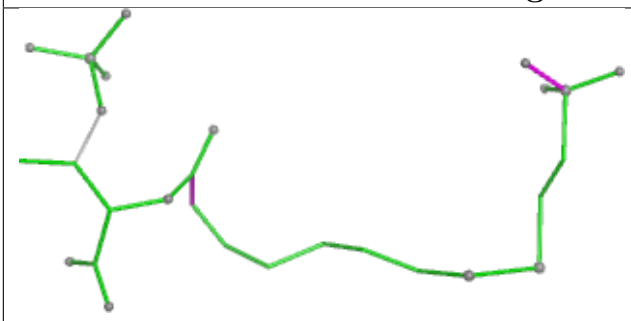


Rings

Ligand SHT E 601



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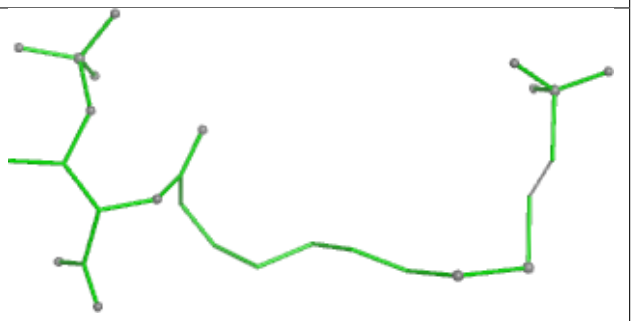

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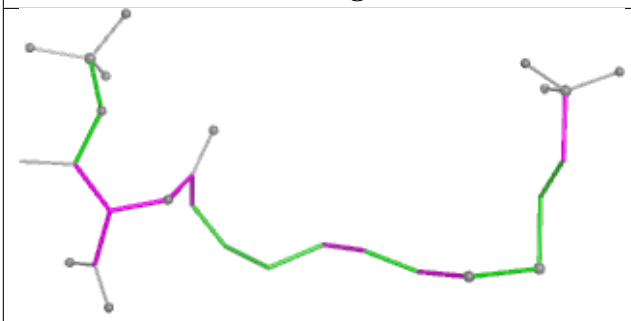

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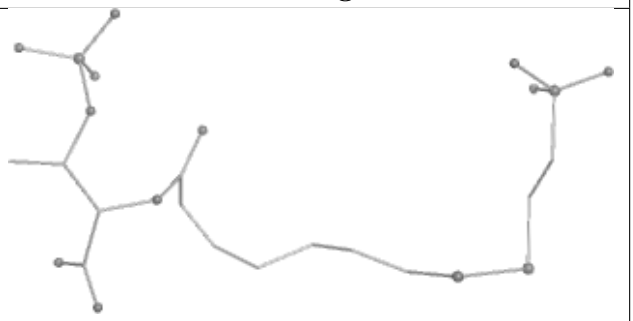
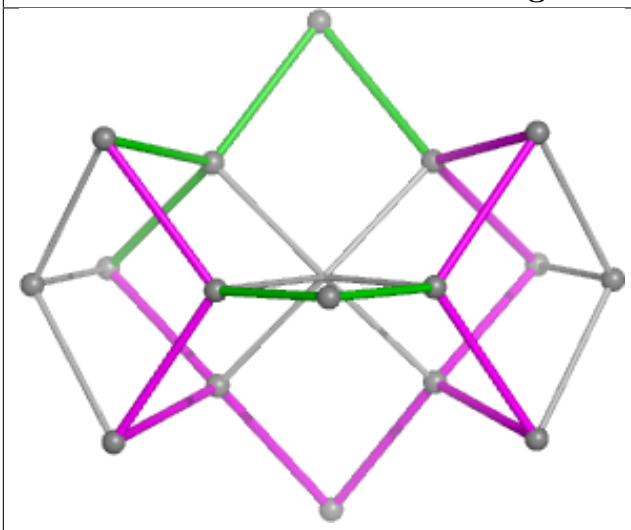
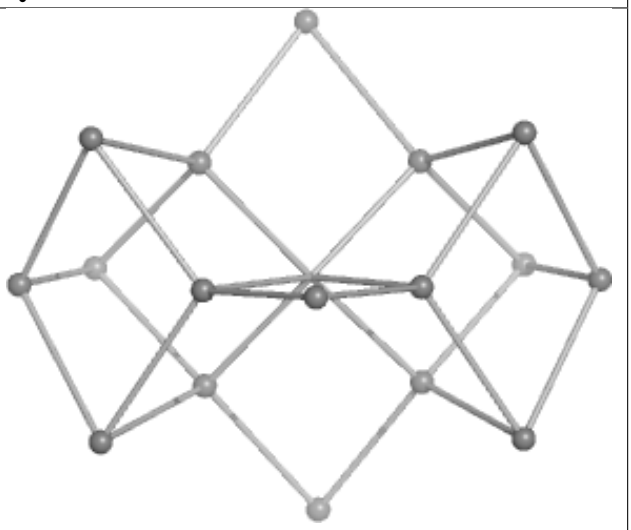


Rings

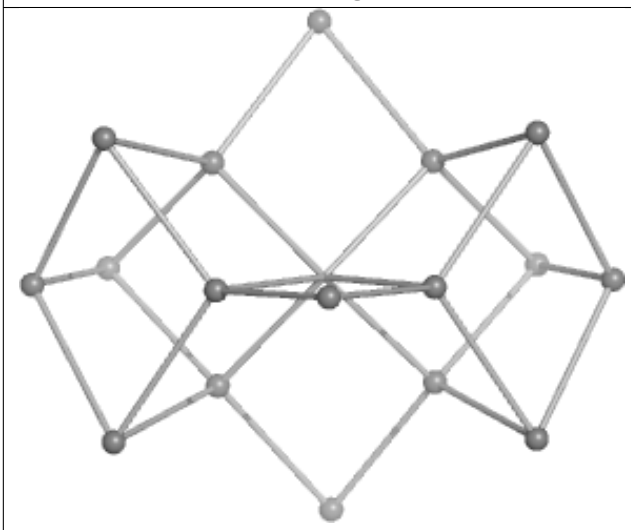
Ligand S5Q H 401



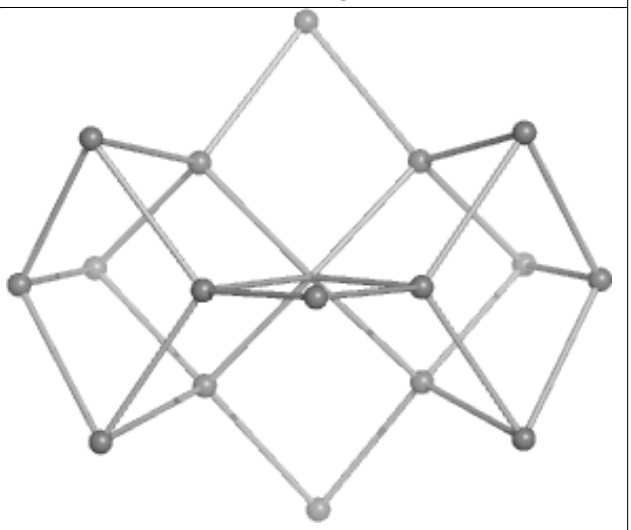
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	4
8	J	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	183:THR	C	184:ASN	N	3.53
1	C	402:SER	C	403:MGN	N	2.98
1	C	403:MGN	C	404:ARG	N	2.95
1	J	22:GLU	C	23:TYR	N	2.59
1	C	447:TYR	C	448:GL3	N	0.84
1	C	448:GL3	C	449:TYR	N	0.47

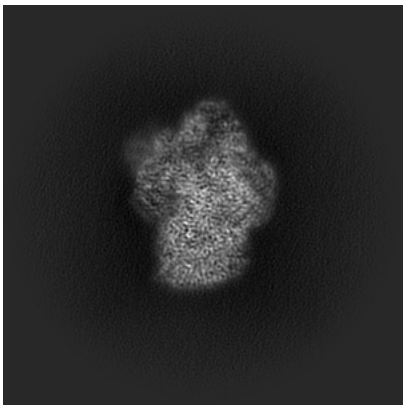
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19787. These allow visual inspection of the internal detail of the map and identification of artifacts.

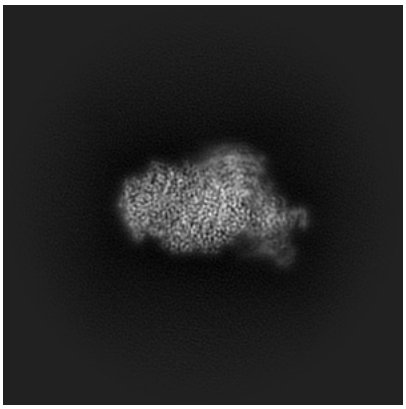
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

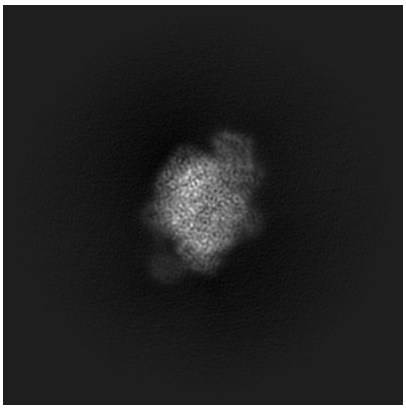
6.1.1 Primary map



X

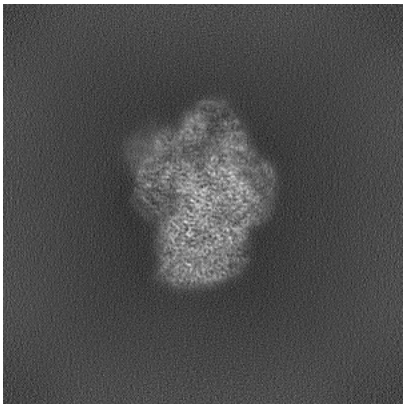


Y

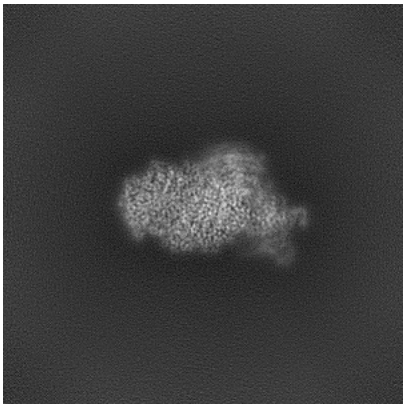


Z

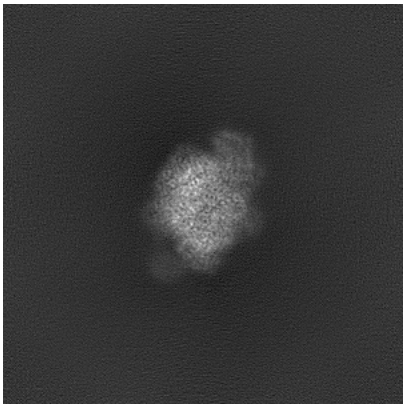
6.1.2 Raw map



X



Y

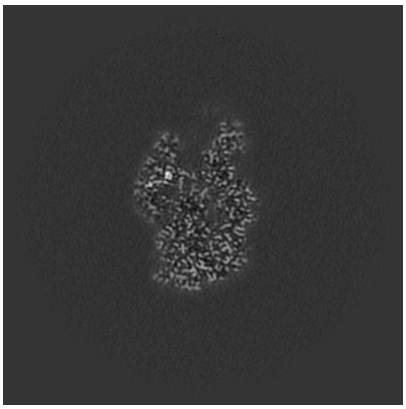


Z

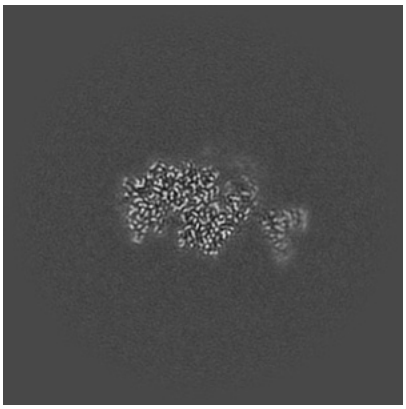
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

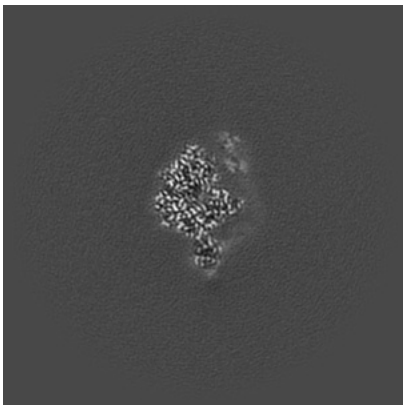
6.2.1 Primary map



X Index: 240

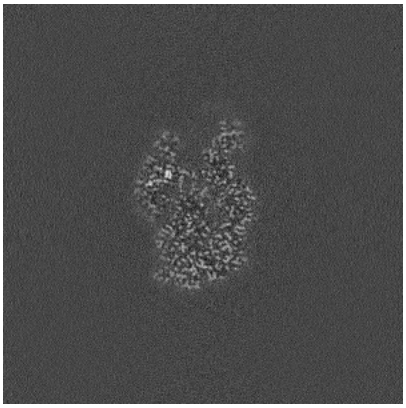


Y Index: 240

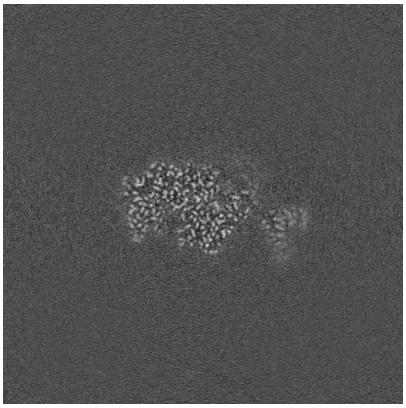


Z Index: 240

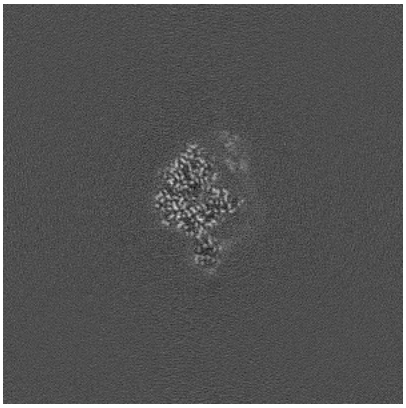
6.2.2 Raw map



X Index: 240



Y Index: 240

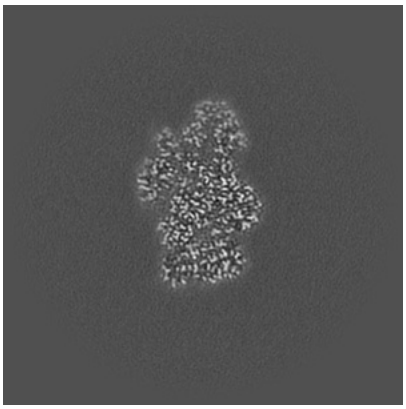


Z Index: 240

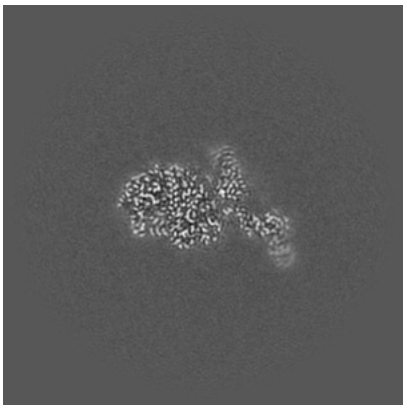
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

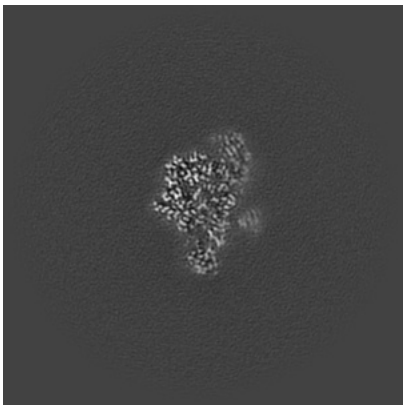
6.3.1 Primary map



X Index: 228

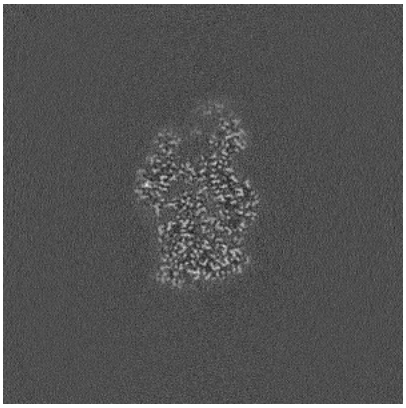


Y Index: 224

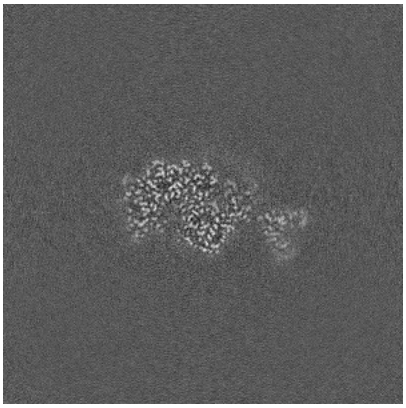


Z Index: 254

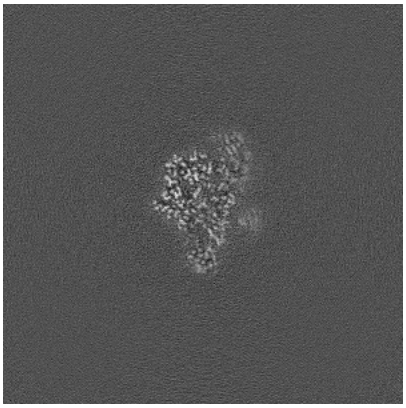
6.3.2 Raw map



X Index: 235



Y Index: 238

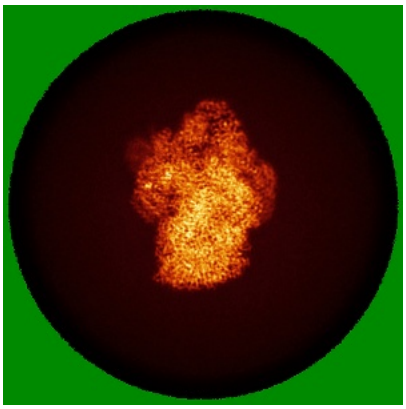


Z Index: 254

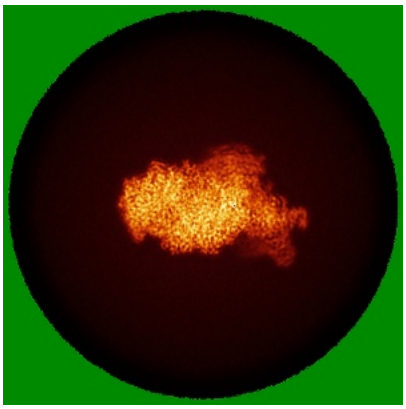
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

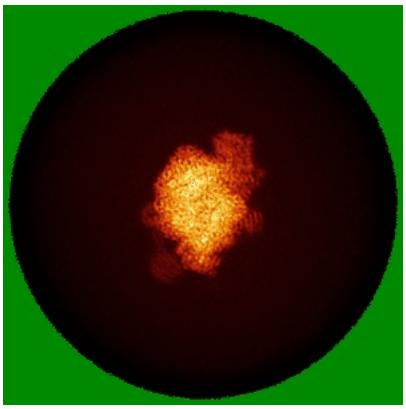
6.4.1 Primary map



X

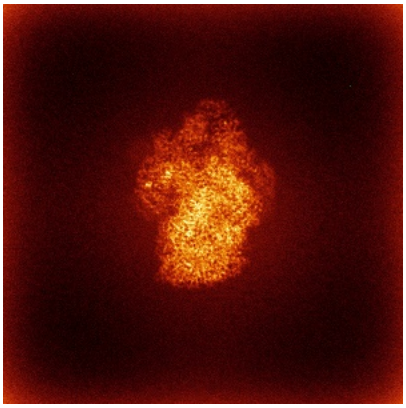


Y

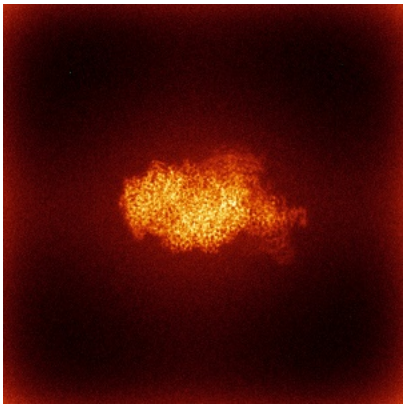


Z

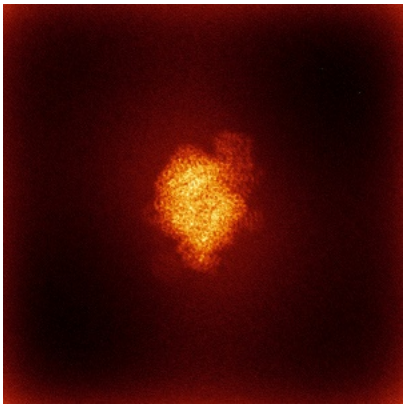
6.4.2 Raw map



X



Y

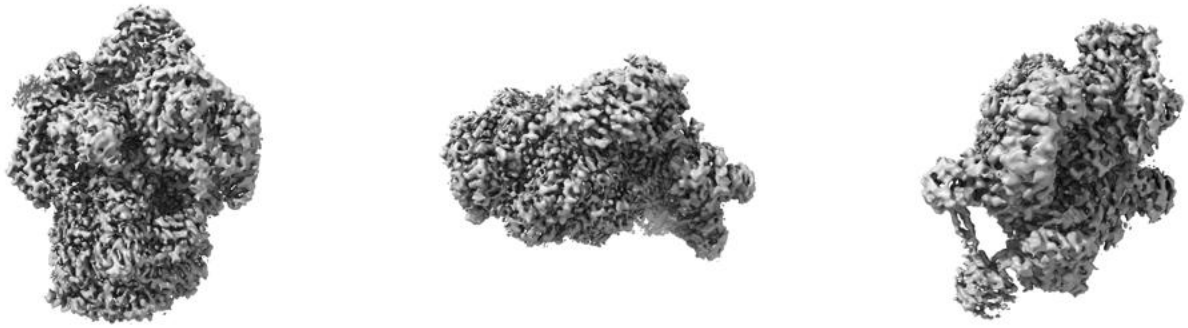


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

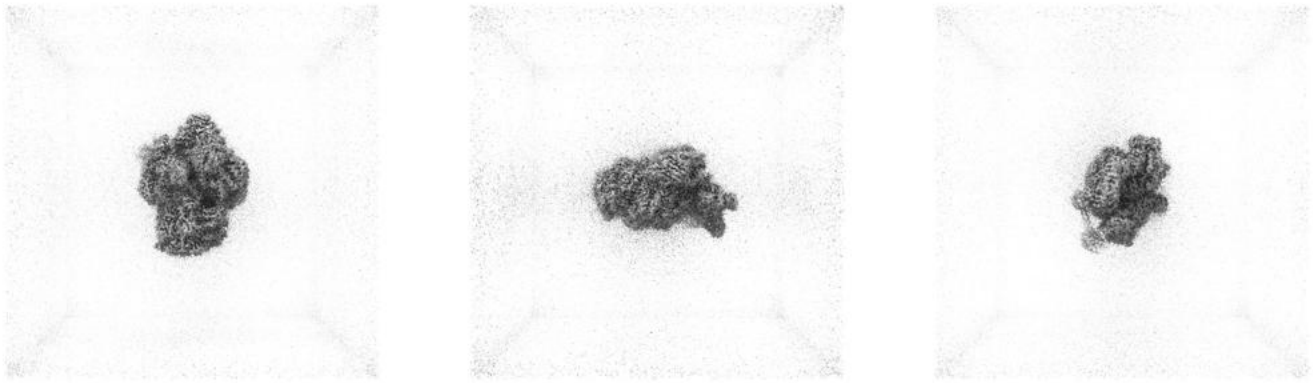
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.051. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

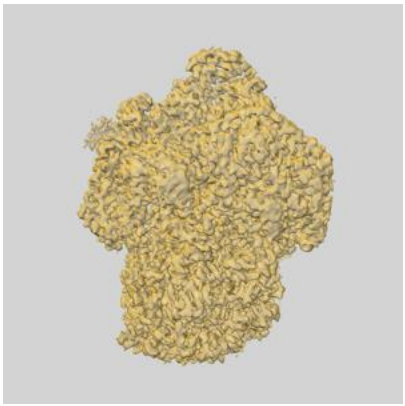
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

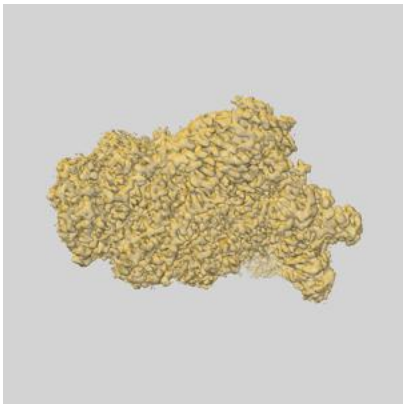
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

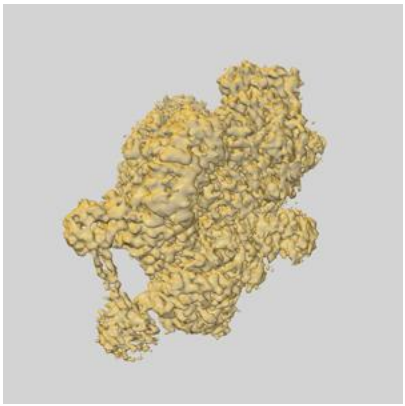
6.6.1 emd_19787_msk_6.map (i)



X

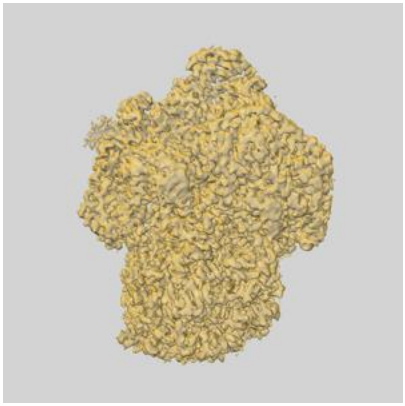


Y

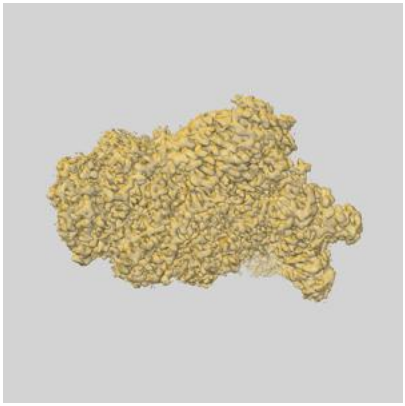


Z

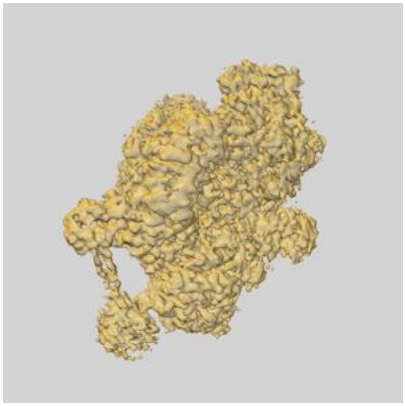
6.6.2 emd_19787_msk_5.map (i)



X

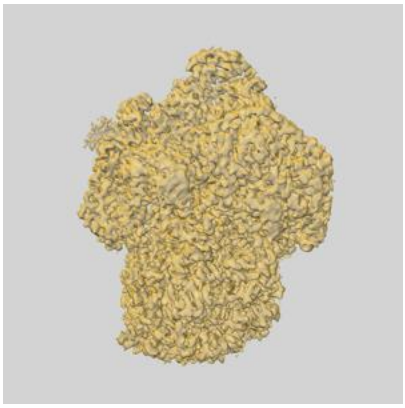


Y

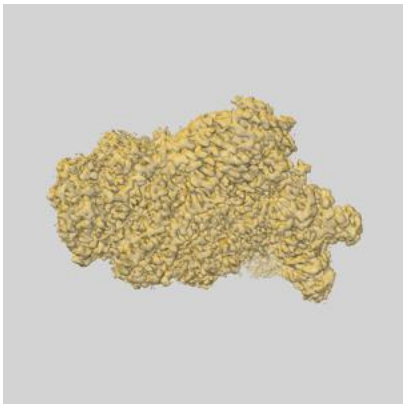


Z

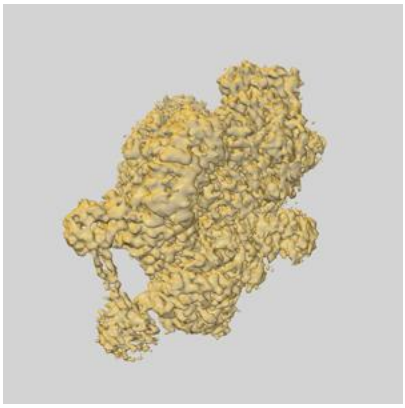
6.6.3 emd_19787_msk_4.map



X

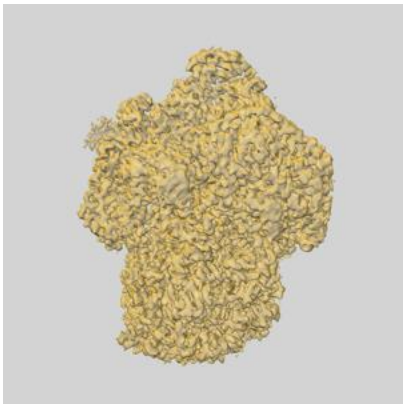


Y

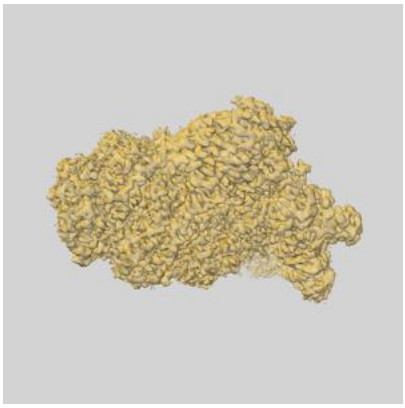


Z

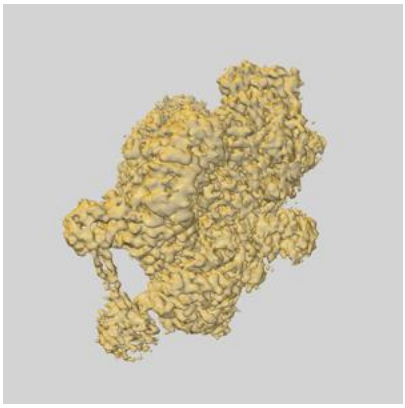
6.6.4 emd_19787_msk_3.map



X

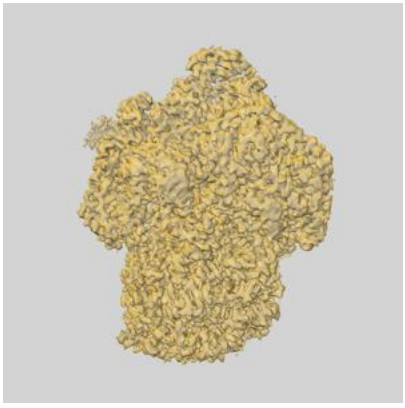


Y

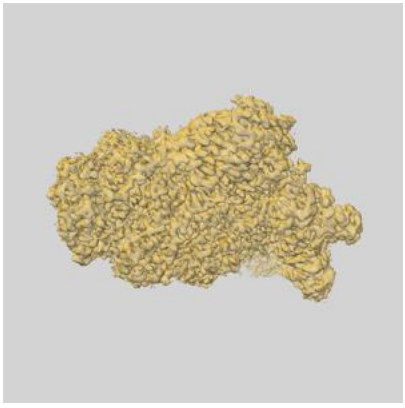


Z

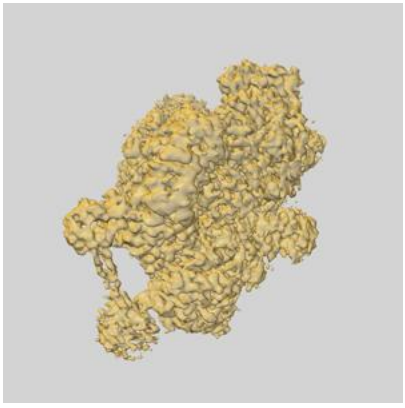
6.6.5 emd_19787_msk_2.map



X

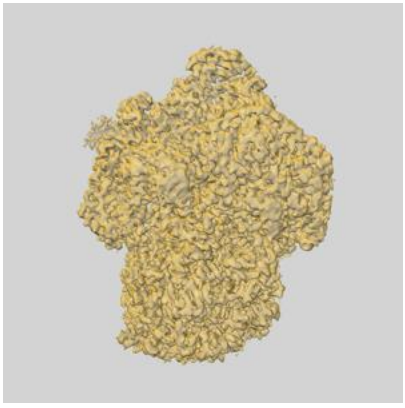


Y

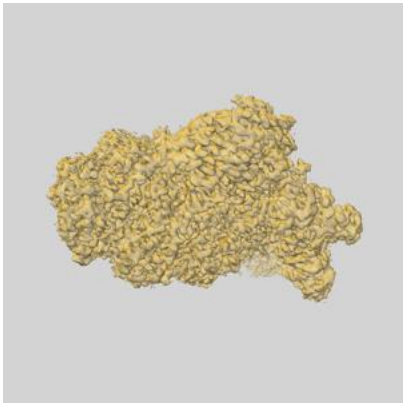


Z

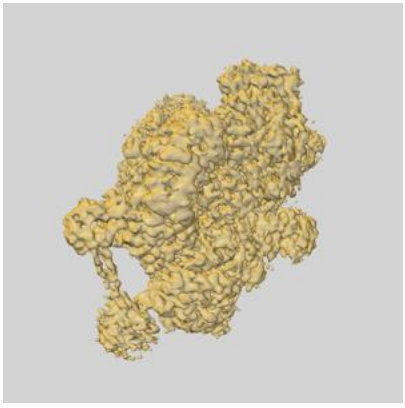
6.6.6 emd_19787_msk_1.map ⓘ



X



Y

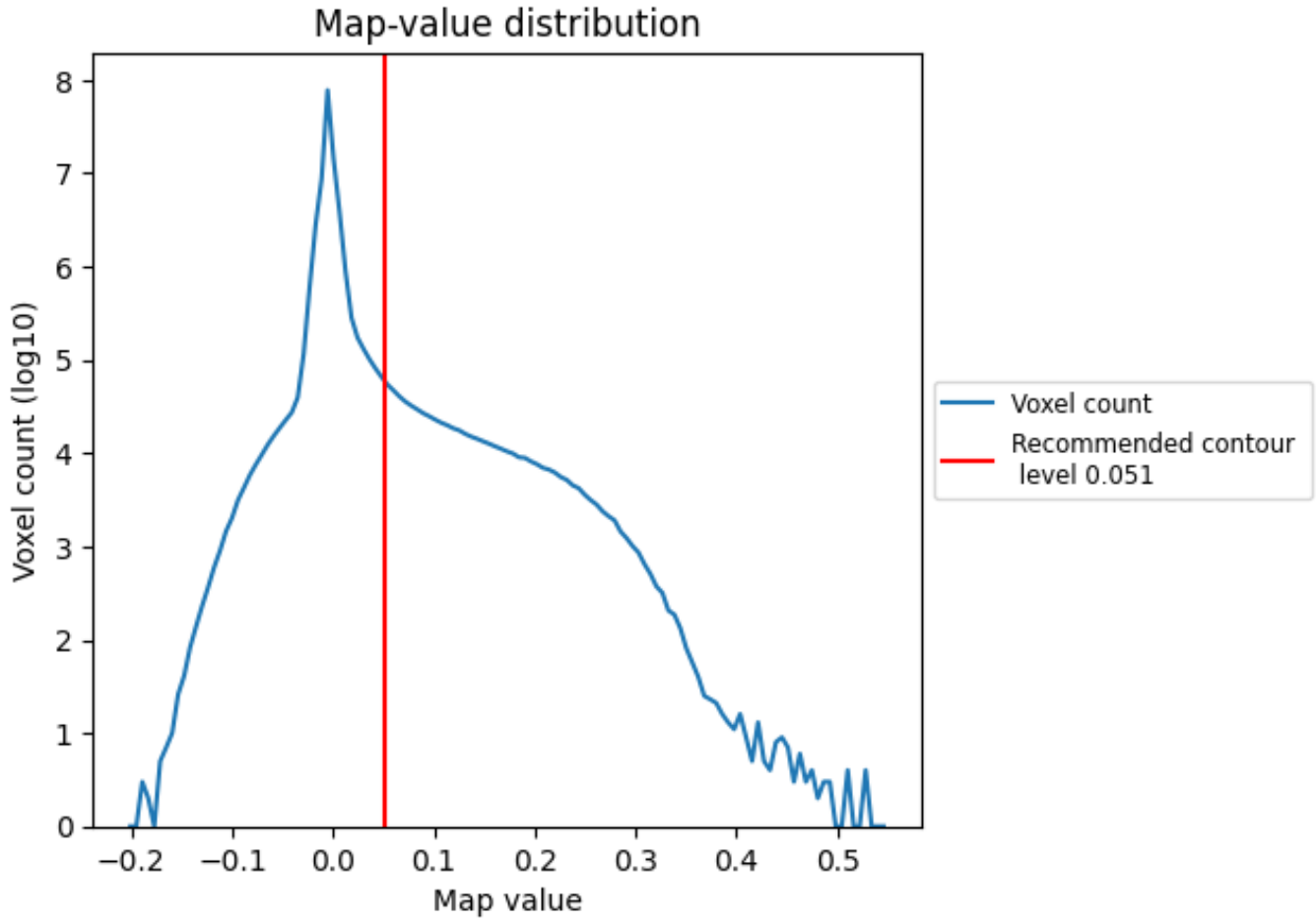


Z

7 Map analysis

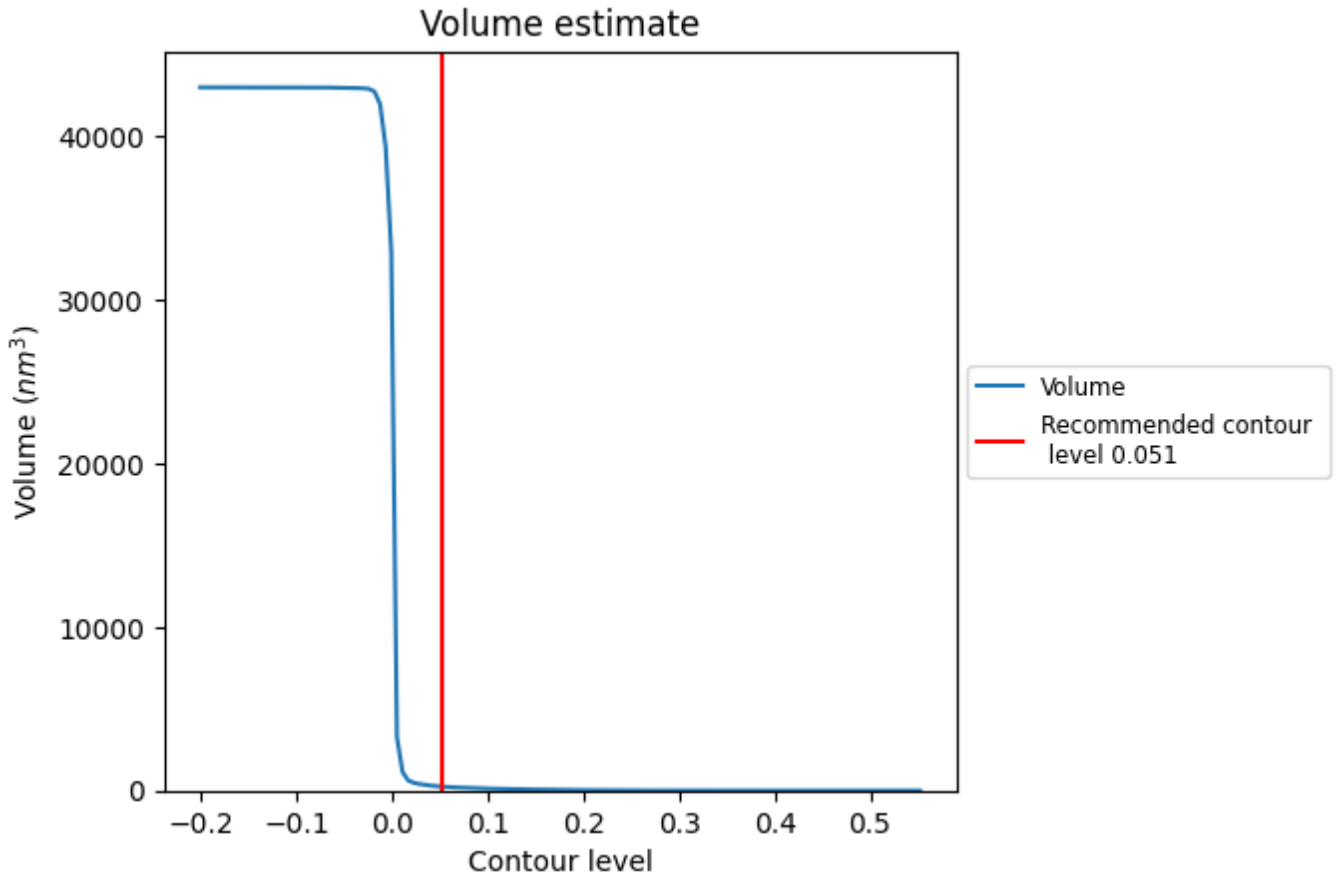
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

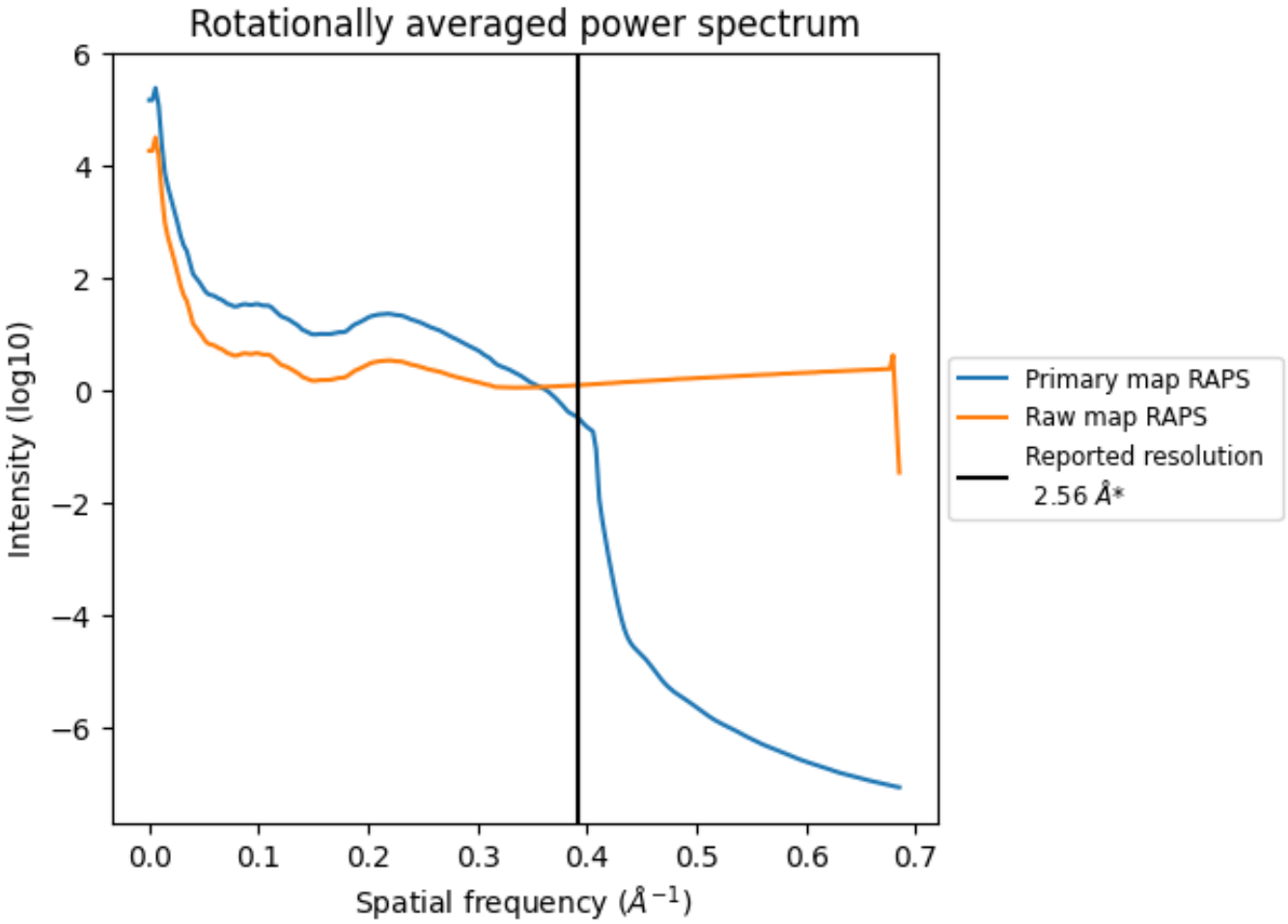
7.2 Volume estimate



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

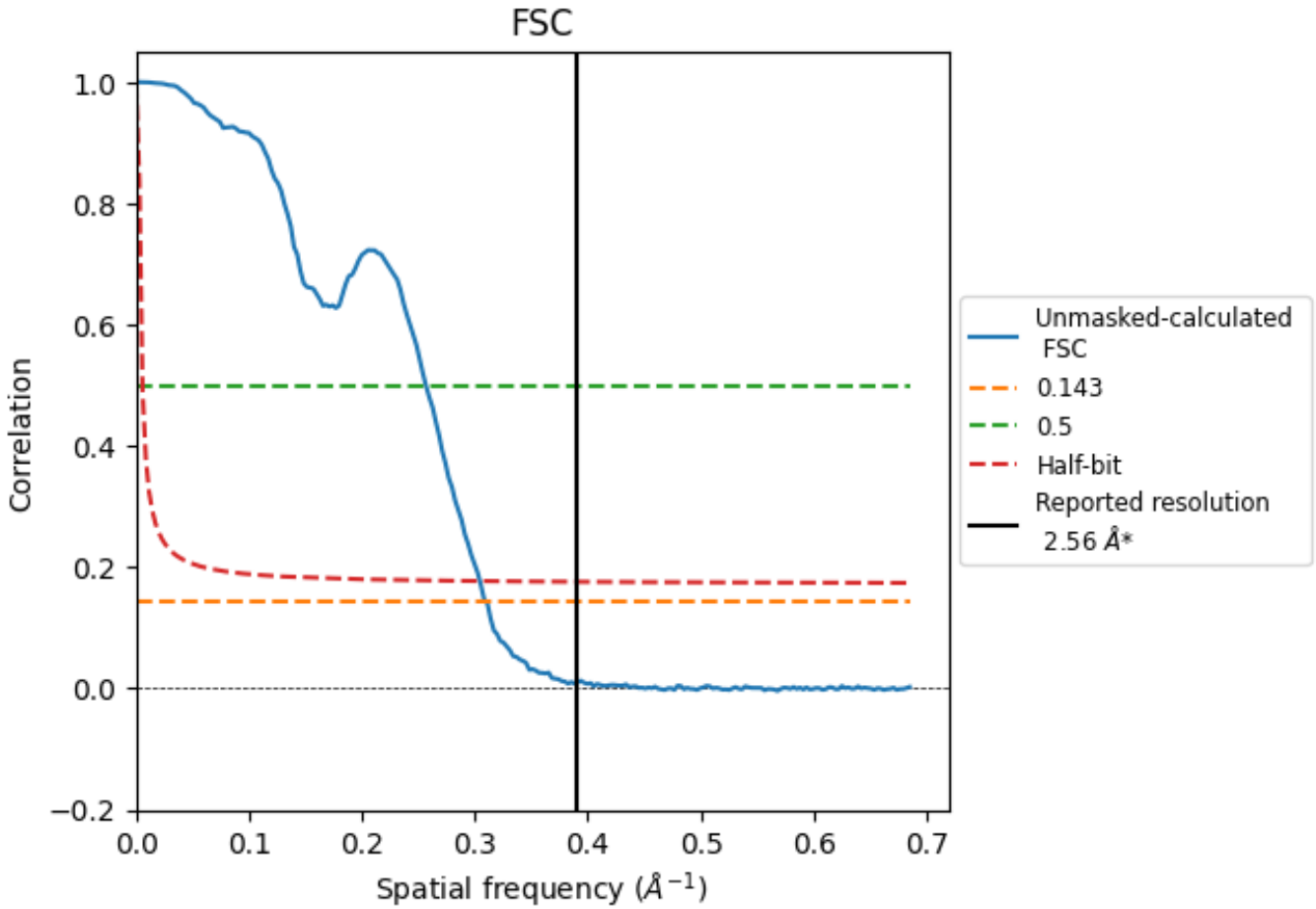


*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8.2 Resolution estimates (i)

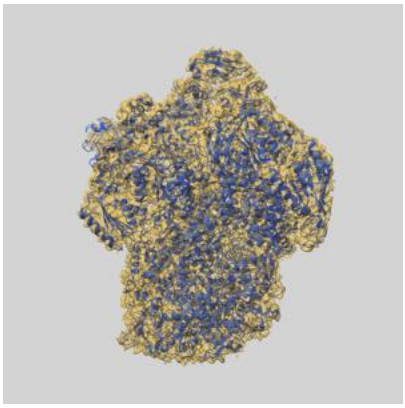
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.90	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.56 by more than 10 %

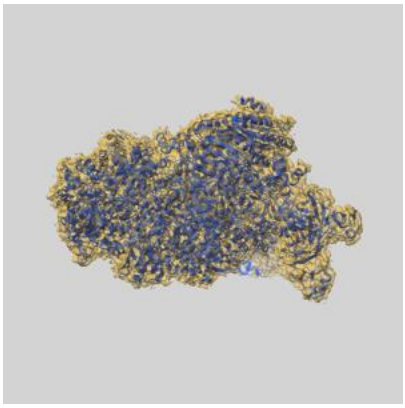
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19787 and PDB model 8S7V. Per-residue inclusion information can be found in section 3 on page 11.

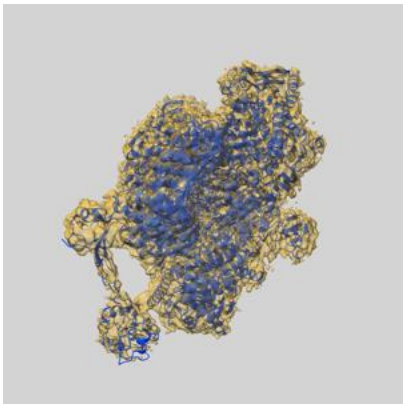
9.1 Map-model overlay



X



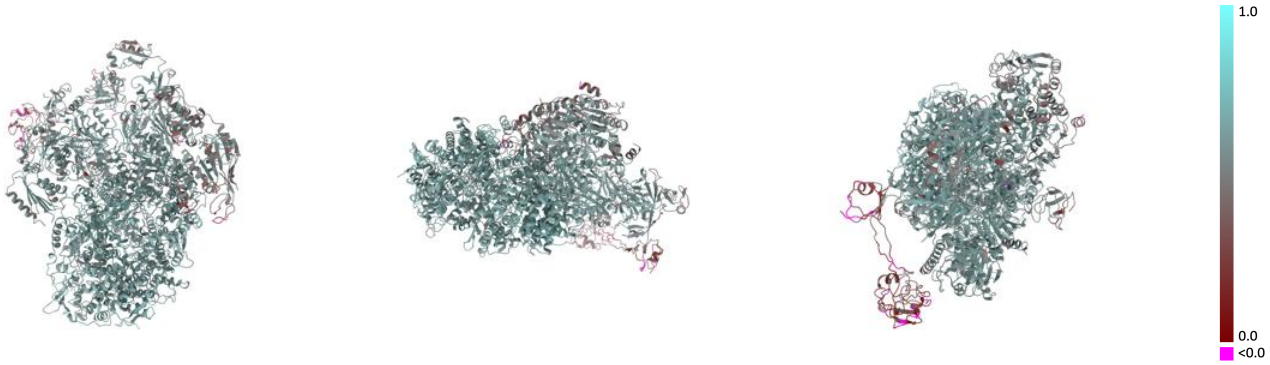
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

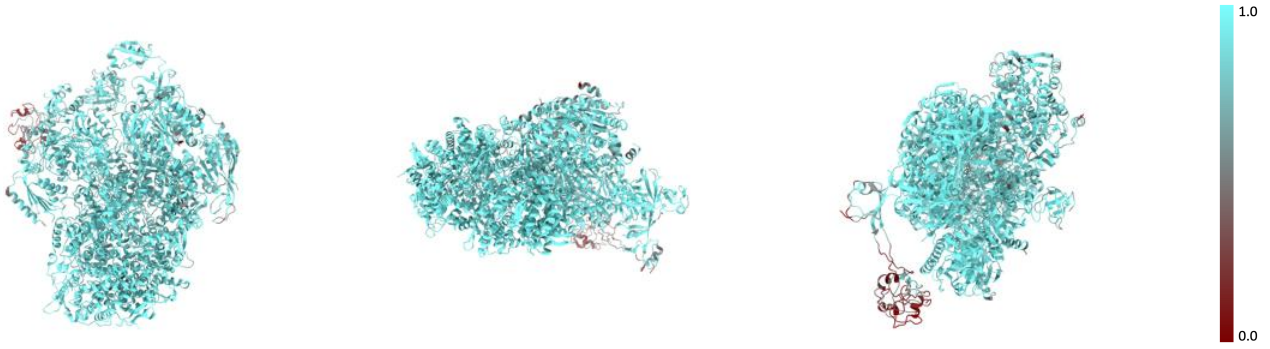
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

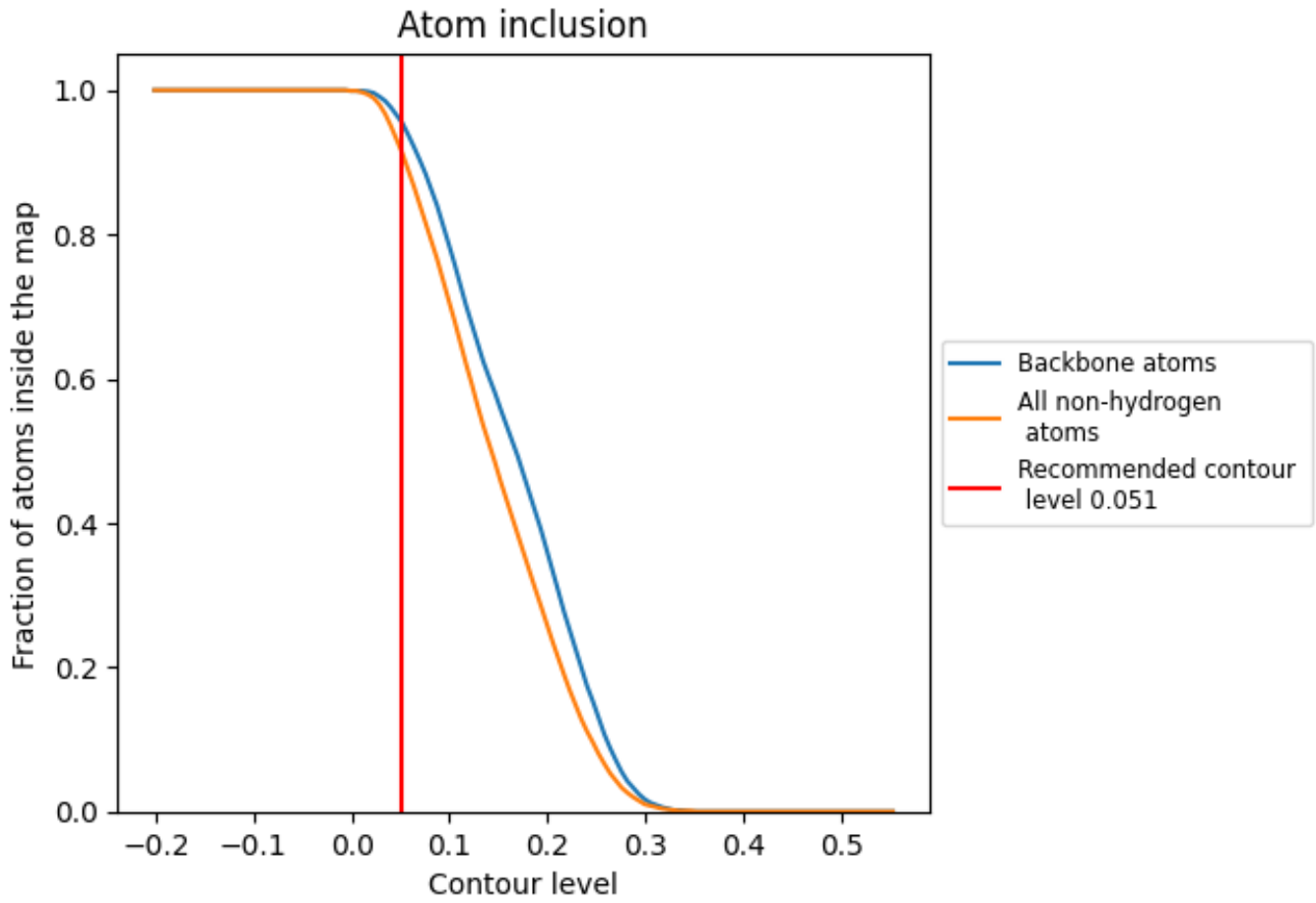
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.051).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.051) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.5690
A	0.9690	0.6060
B	0.9670	0.6270
C	0.9710	0.6160
D	0.9800	0.6150
E	0.9730	0.6160
F	0.9650	0.6150
G	0.9100	0.5640
H	0.9350	0.5690
I	0.9410	0.5860
J	0.7070	0.4180
K	0.8500	0.5050
L	0.8240	0.4580